

*Probing buried solid-solid and solid-liquid interfaces
with standing-wave-excited spectroscopies:
photoemission (well along) and soft x-ray emission and
resonant elastic/inelastic scattering (just beginning)*



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Bunkyo-ku, Tokyo, Japan

⁸Donostia International Physics Center,
San Sebastian, Spain

⁹Hirosaki University, Japan

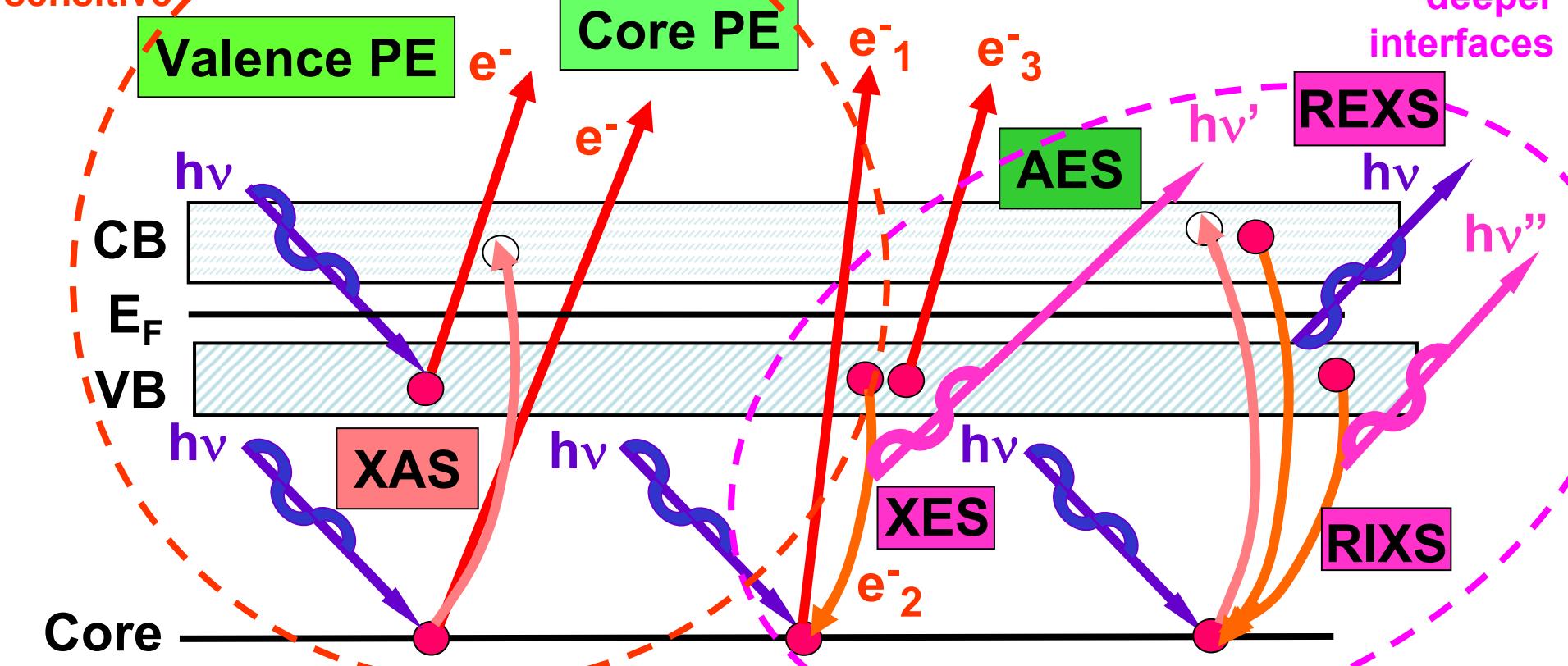


The Advanced
Light Source

Outline

- Experimental aspects– end station on beamline 4.0.2
- Standing wave basics—rocking curves and wedges
- Photon-in/electron-out studies of spintronic nanolayer structures
- Photon-in/photon-out studies of spintronic nanolayer structures
- Future possibilities with photon-in/photon-out, including gas-solid and liquid-solid interfaces
- Resonant elastic soft x-ray scattering from nanostructures: Toward soft x-ray photonics?

The Soft X-Ray Spectroscopies



PE = photoemission = photoelectron spectroscopy

XAS = x-ray absorption spectroscopy

AES = Auger electron spectroscopy

XES = x-ray emission spectroscopy

REXS/RIXS = resonant elastic/inelastic x-ray scattering

Red =
developments
in progress

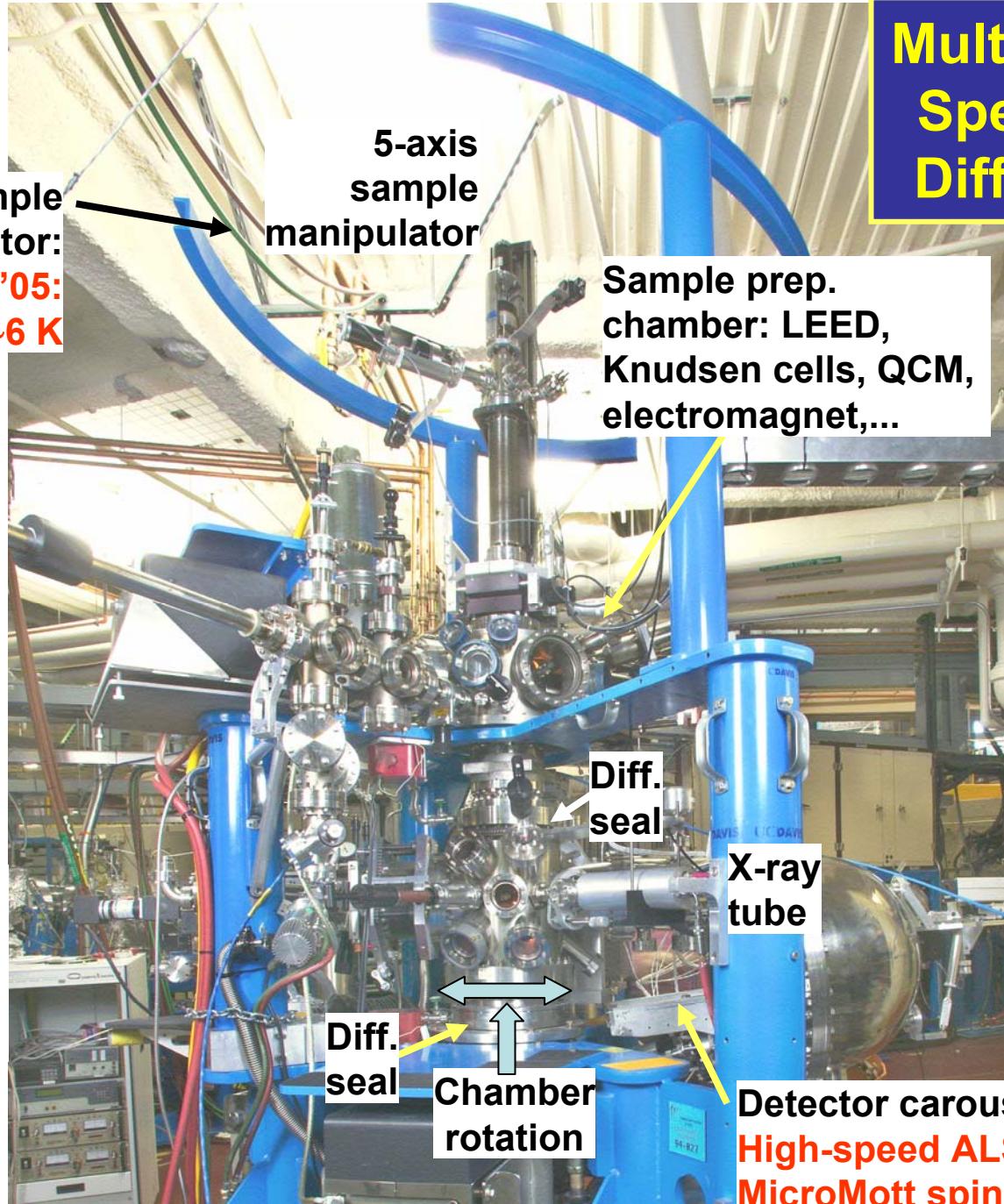
Sample
manipulator:

To be replaced '05:
T down to ~6 K

Loadlock
for sample
introduction

Refocussing
mirror ('05-06)

Soft x-ray
spectrometer:
Scienta
XES 300



Multi-Technique Spectrometer/ Diffractometer

Permits using all relevant soft x-ray spectroscopies on a single sample: PS, PD, PH; XAS (e^- or photon detection), XES/REXS/RIXS, with MCD, MLD

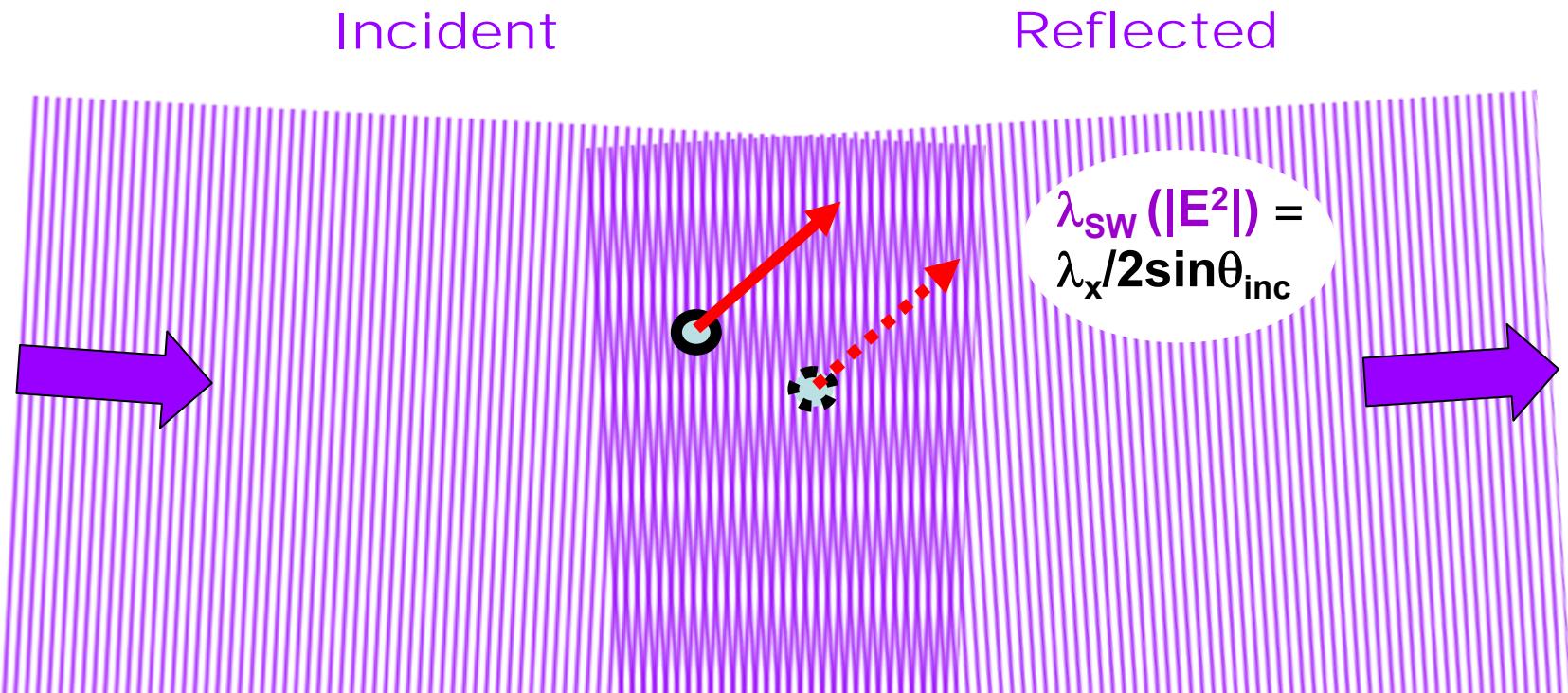
Electron spectrometer:
Scienta SES 200
Power supply upgrade ('05-'06)

Detector carousel:
High-speed ALS detector ('05) + MicroMott spin detector ('05)

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Standing wave formation in reflection from a surface, or single-crystal Bragg planes⁺, or a multilayer mirror



If incident angle = reflected angle (specular reflection)
standing wave is parallel to surface

⁺Bragg reflection of hard x-rays:
Batterman, Phys. Rev A 133, 759 (1964)

Standing wave formation:

$$I_{sw}(|E^2|) \propto |\phi_{inc} + \phi_{refl}|^2$$
$$= |\phi_{inc}|^2 + \underbrace{\phi_{inc}\phi_{refl}^* + \phi_{inc}^*\phi_{refl}}_{+ |\phi_{refl}|^2} + |\phi_{refl}|^2$$

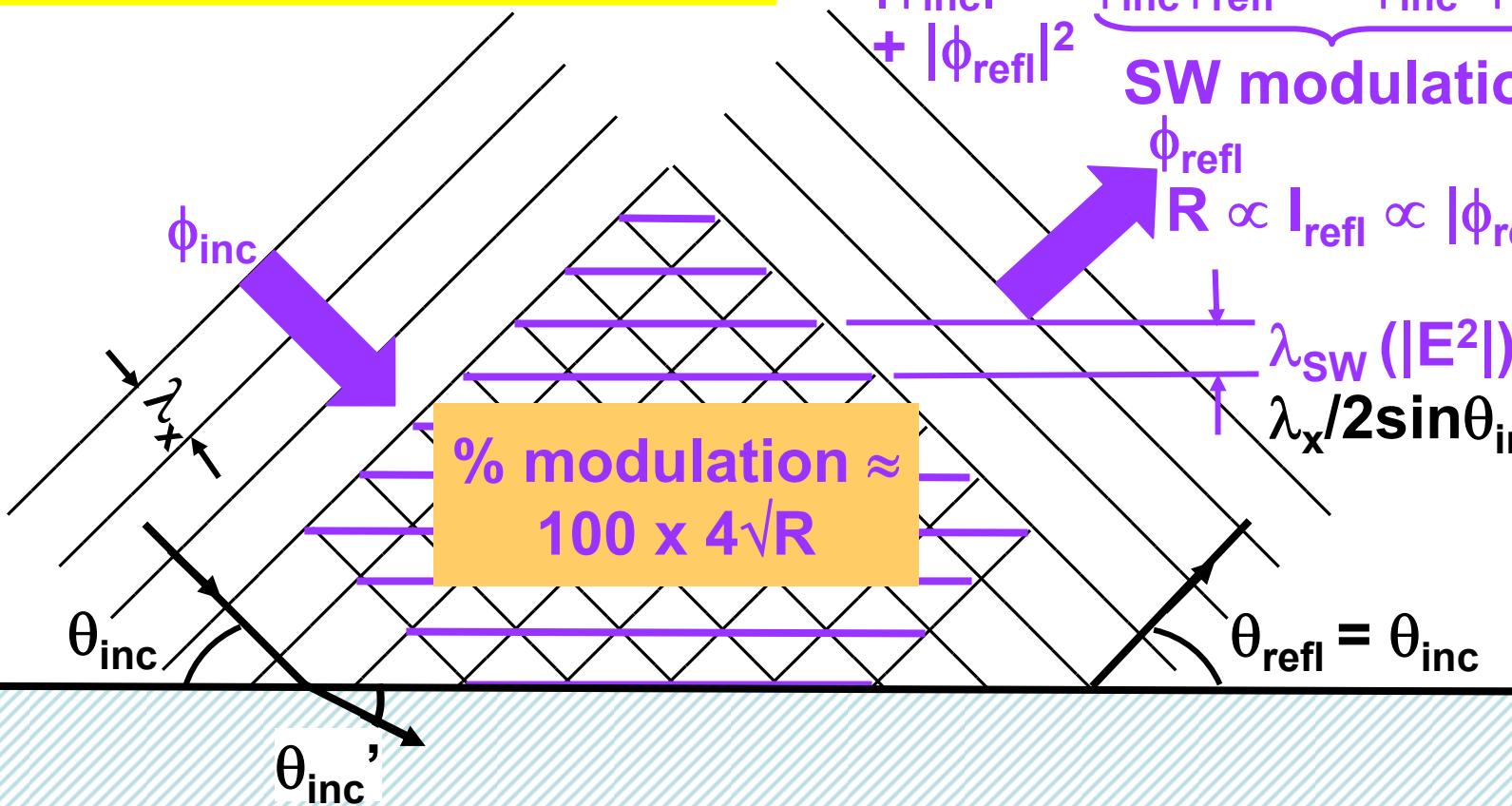
SW modulation

ϕ_{refl}

$$R \propto I_{refl} \propto |\phi_{refl}|^2$$

$$\lambda_{sw}(|E^2|) = \lambda_x / 2 \sin \theta_{inc}$$

% modulation \approx
 $100 \times 4\sqrt{R}$



- $n(h\nu) =$

$$1 - \delta(h\nu) + i\beta(h\nu)$$

- variable polarization

- multiple reflection/refraction

- exact treatment of interlayer intermixing a/o roughness

- electric field at i -th layer:

$$|E_{sw,i}(z)|^2 = |E_i^+(z) + E_i^-(z)|^2$$

Photoemission:

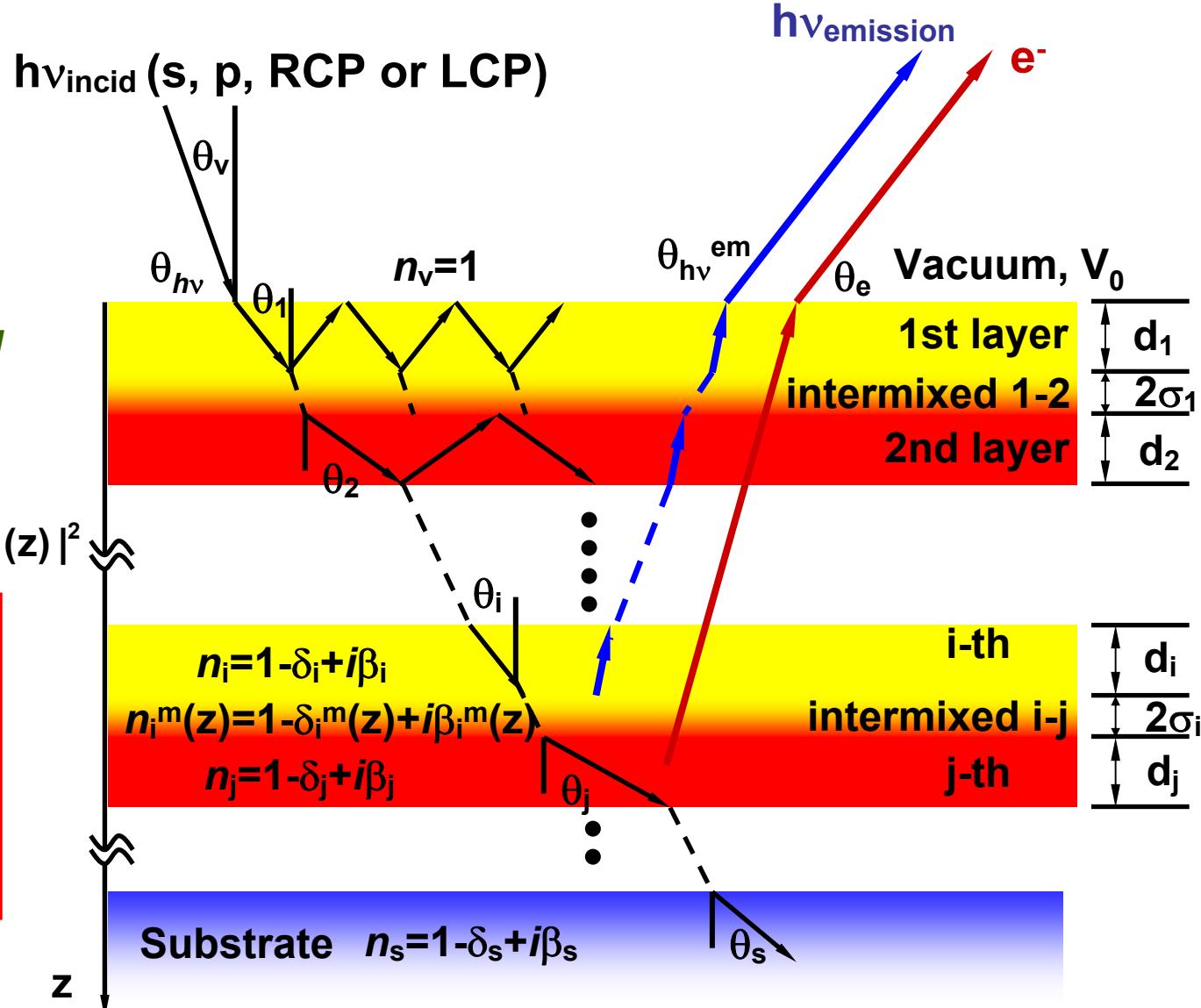
- differential cross section

- inelastic attenuation

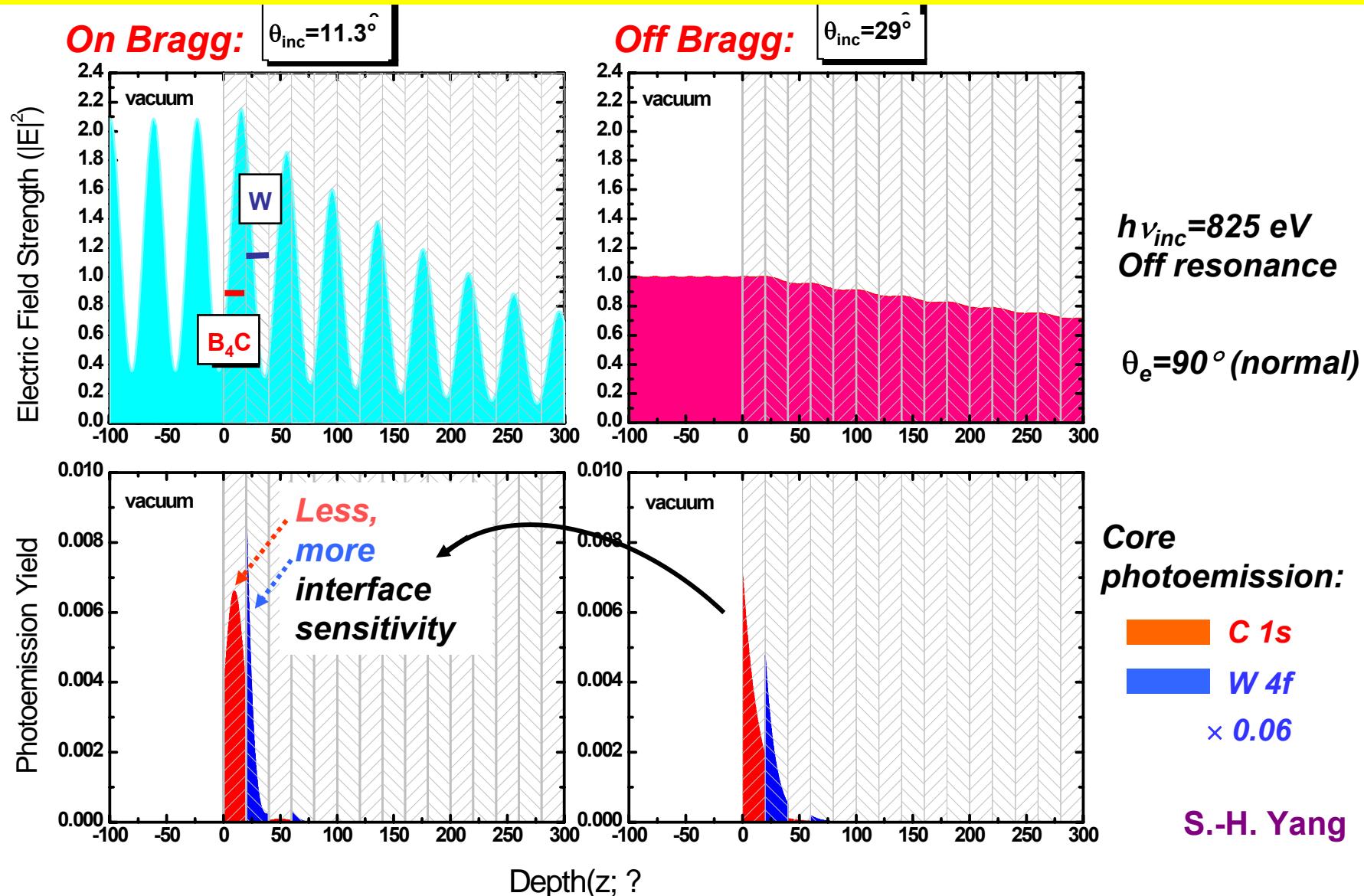
- surface refraction

X-ray emission:

- fluorescence yield



CALCULATED PHOTOEMISSION FROM A MULTILAYER STANDING WAVE GENERATOR (SWG)-- $[B_4C\text{ (20 \AA) /W\text{ (20 \AA)}]_{20}$ /Si



→ Mean depth in photoemission changes with standing wave excitation

- $n(h\nu) =$

$$1 - \delta(h\nu) + i\beta(h\nu)$$

- variable polarization

- multiple reflection/refraction

- exact treatment of interlayer intermixing a/o roughness

- electric field at i -th layer:

$$|E_{sw,i}(z)|^2 = |E_i^+(z) + E_i^-(z)|^2$$

Photoemission:

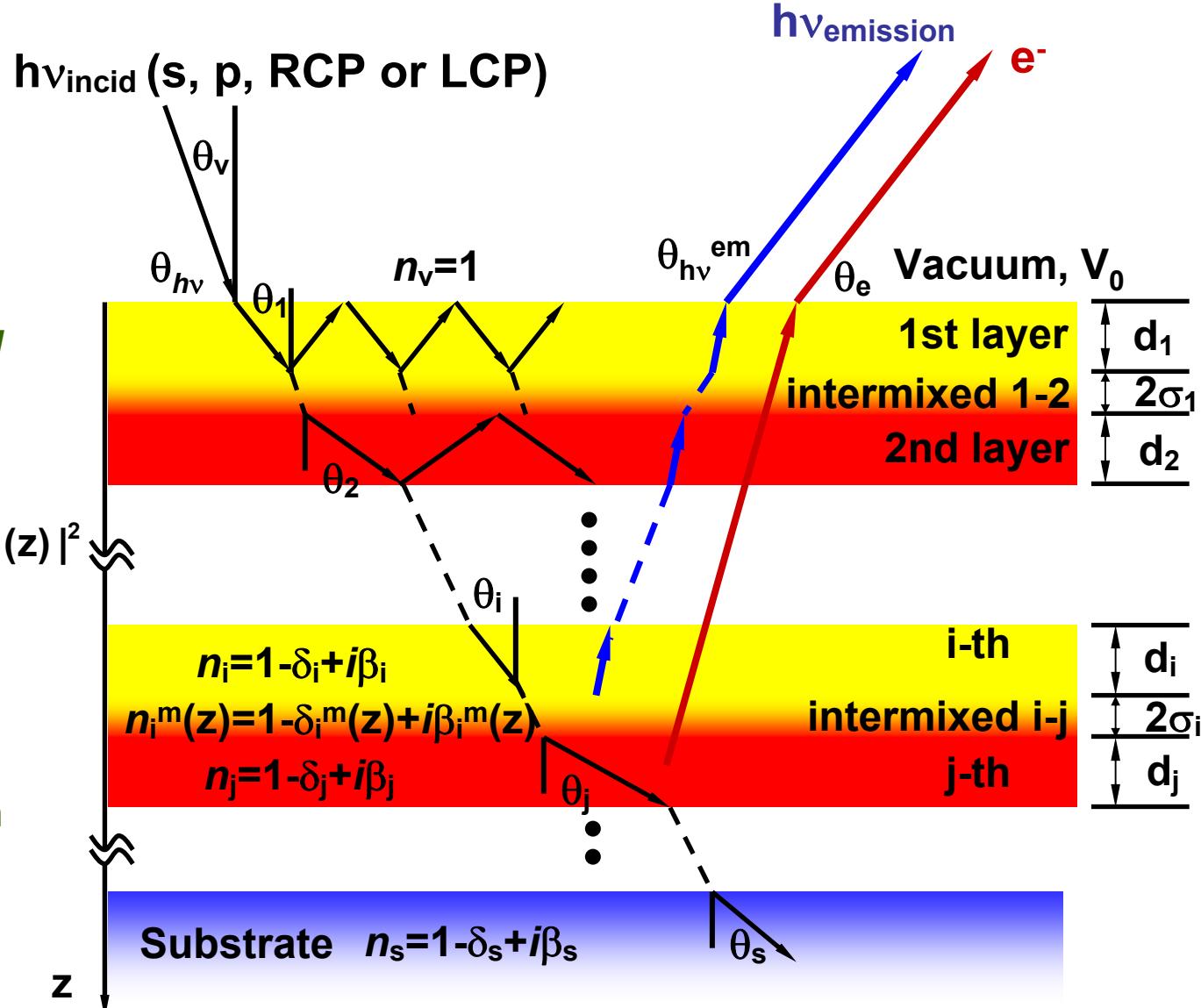
- differential cross section

- inelastic attenuation

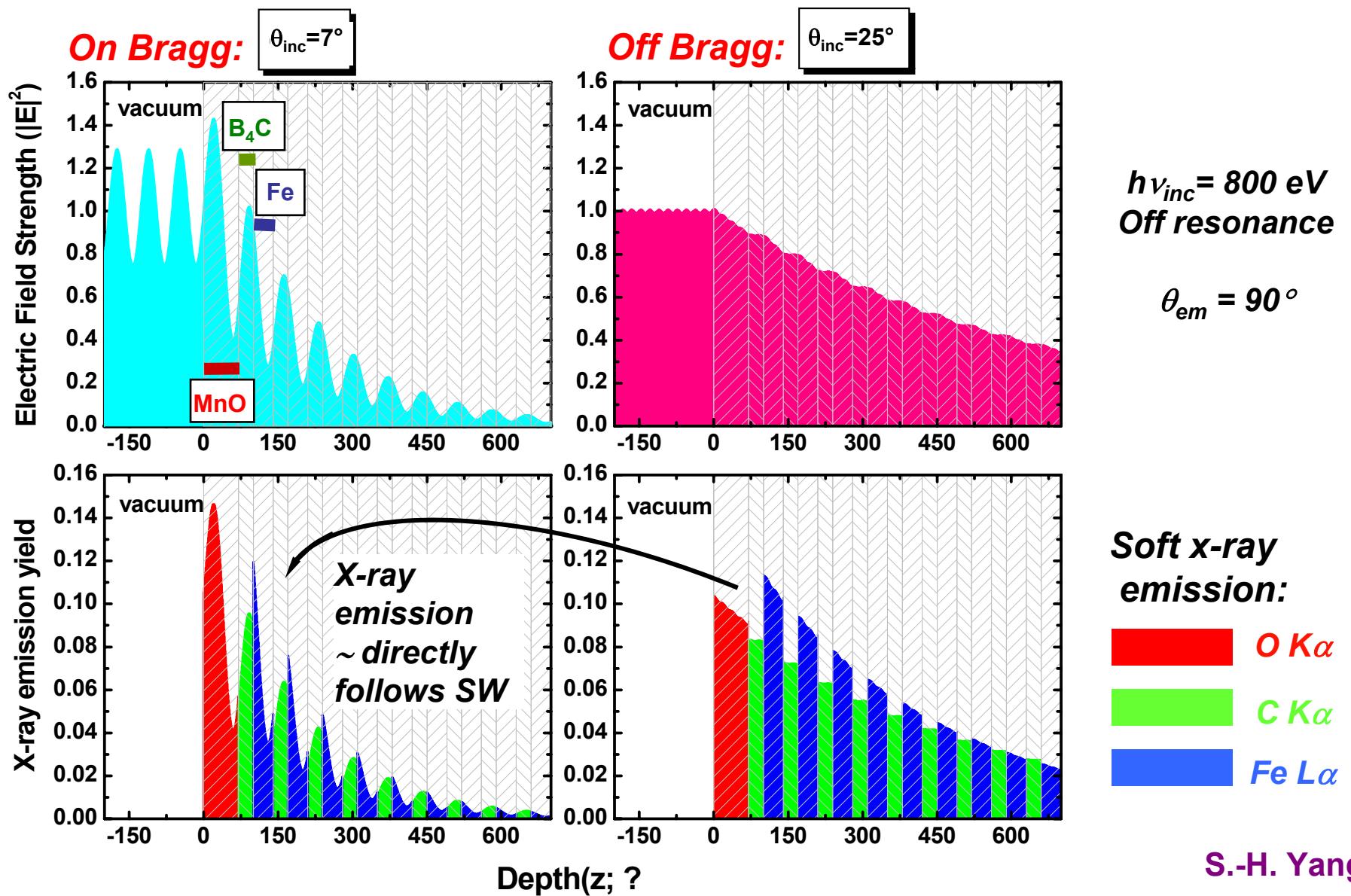
- surface refraction

X-ray emission:

- fluorescence yield



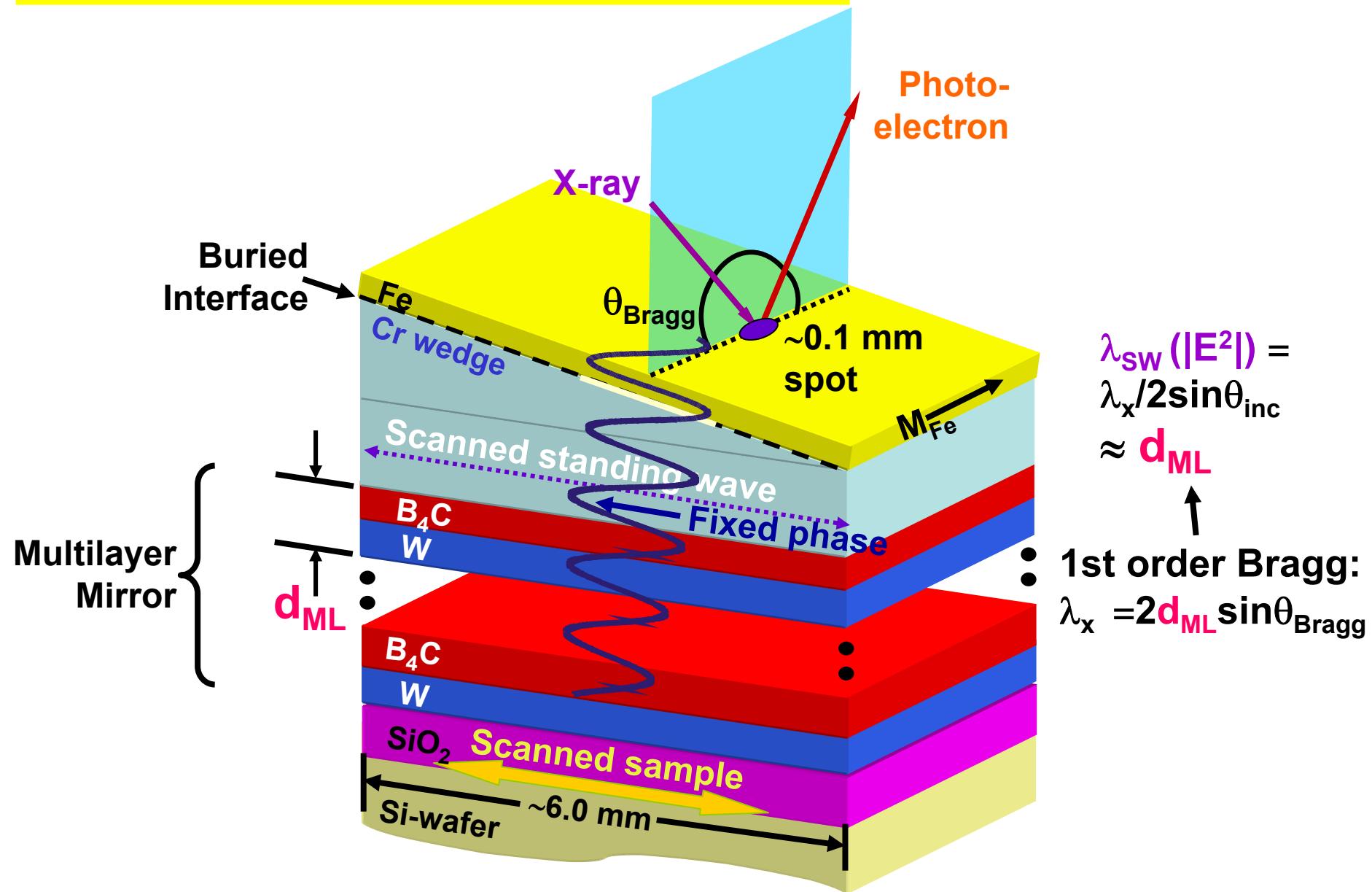
CALCULATED SOFT X-RAY EMISSION FROM A MULTILAYER STANDING WAVE GENERATOR (SWG)-- $MnO(70\text{\AA})/[B_4C(30\text{\AA})/Fe(40\text{\AA})]_{20}/Si$



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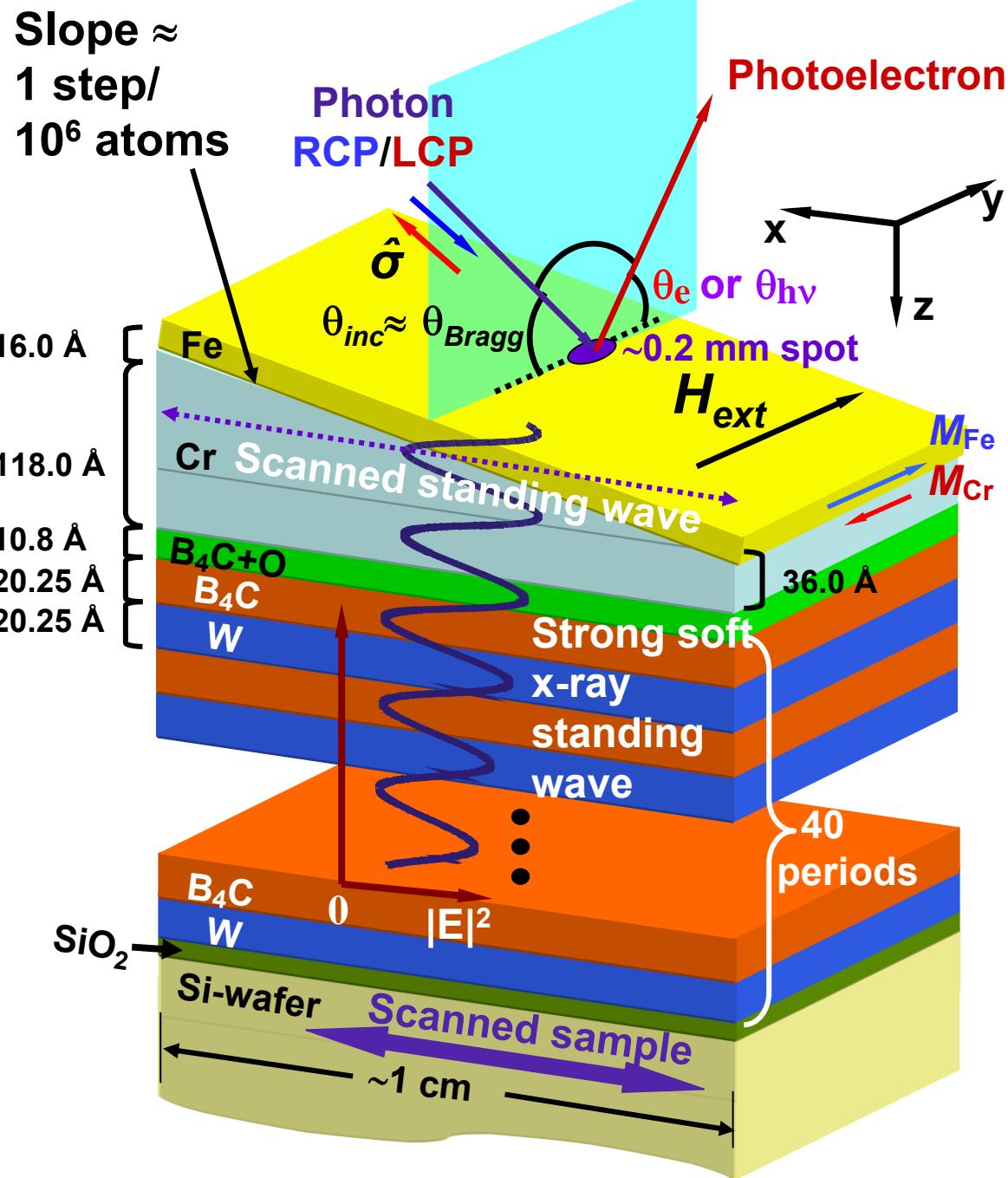
Probing Buried Interfaces: The Standing Wave-Wedge Method



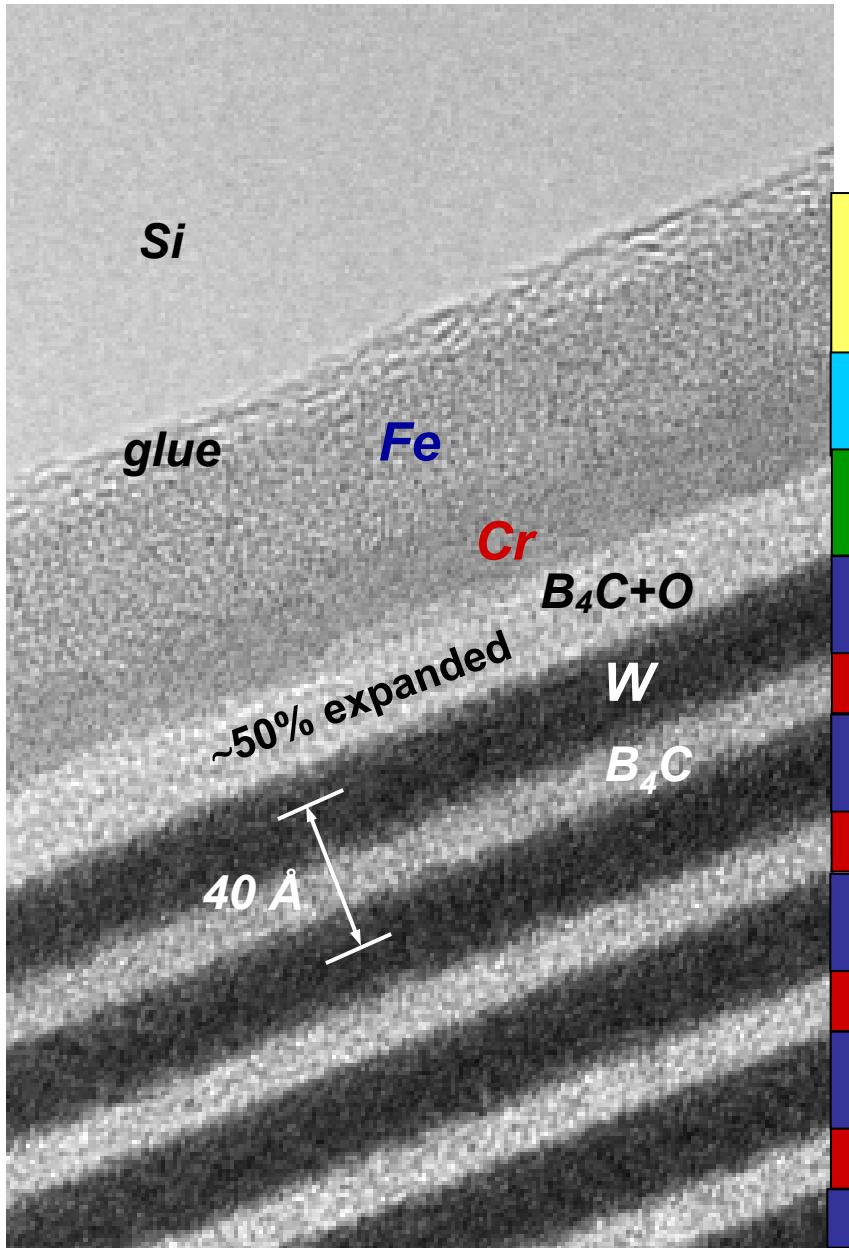
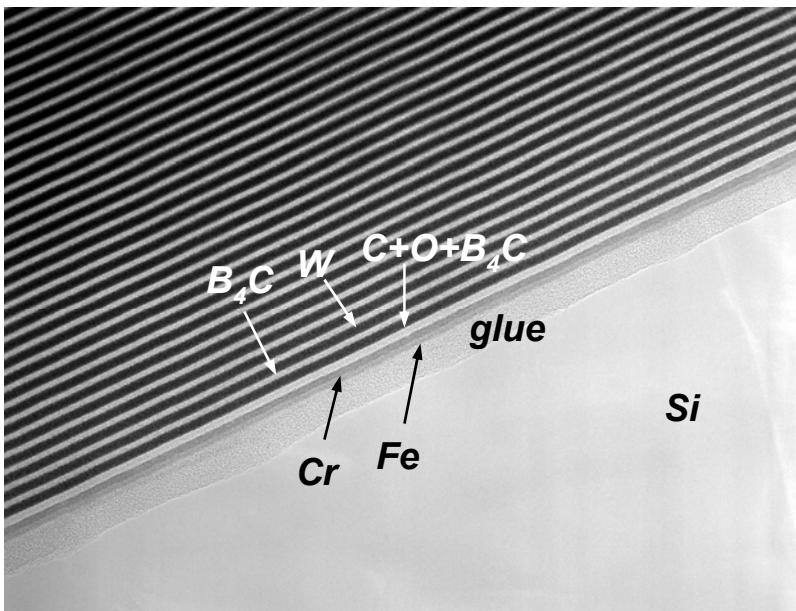
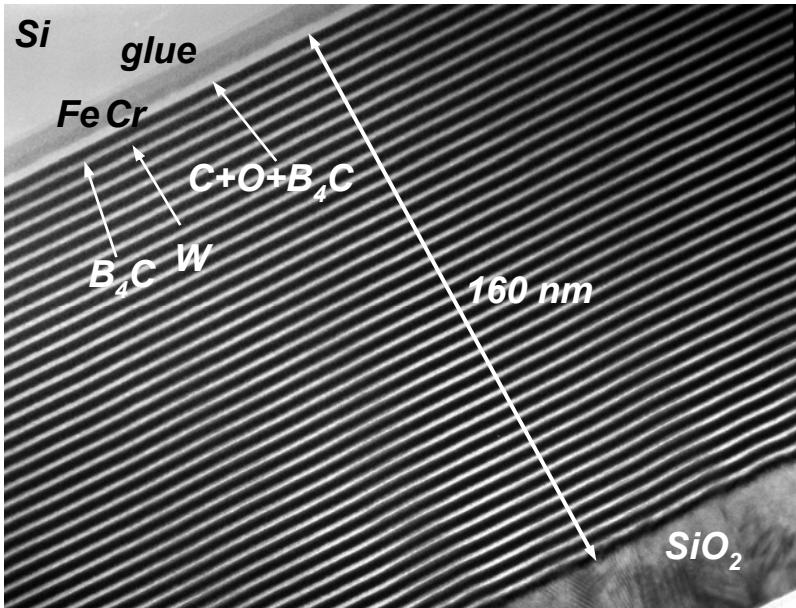
Probing Buried Interfaces with Soft X-ray Standing Waves: Core PS Spectra

Fe/Cr: a prototypical system for giant magneto-resistance

40.50 Å period =
standing wave period



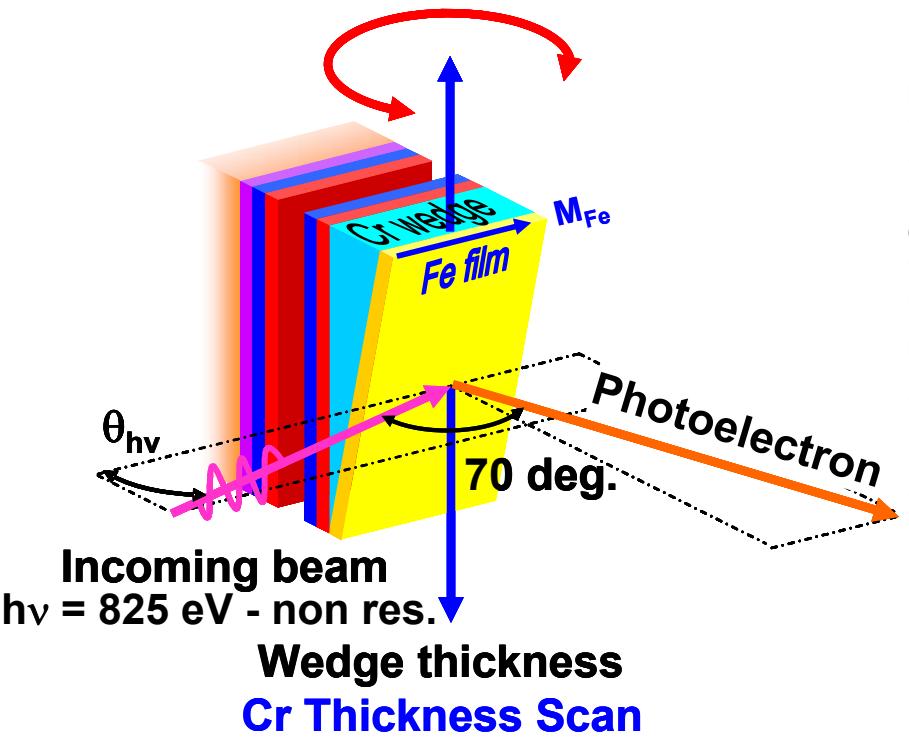
**TRANSMISSION ELECTRON MICROSCOPY IMAGE FOR Fe/Cr/MULTILAYER SWG
(Synthesis-CXRO, and Imaging-NCEM, LBNL)**



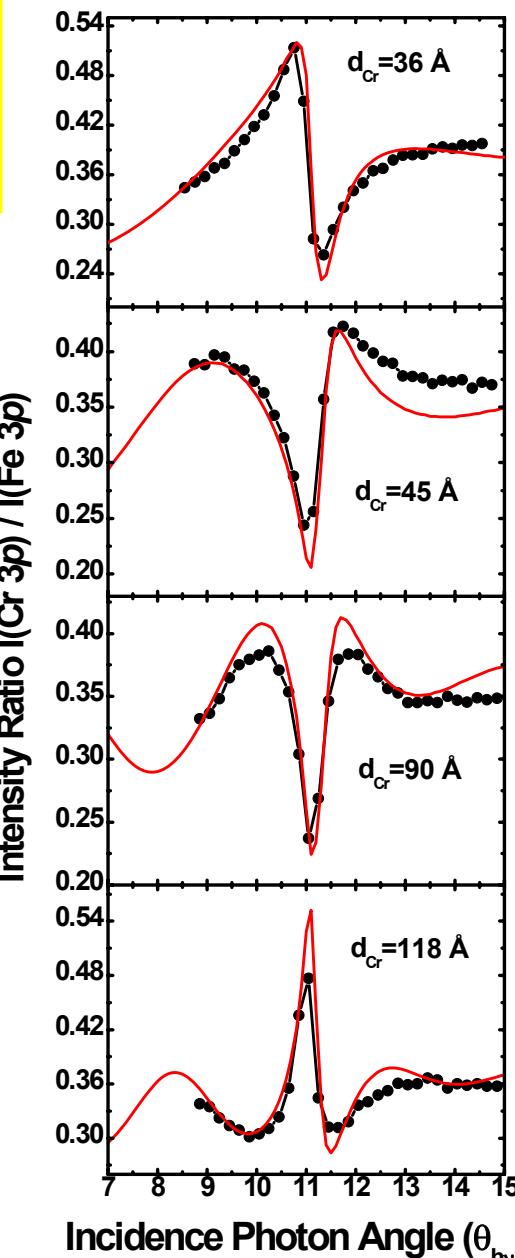
*Experimental + Calculated
Photoemission Yield Ratio
 $I(Fe\ 3p)/I(Cr\ 3p)$ from Fe/Cr wedge
on standing-wave multilayer*

Incidence Photon Angle Scan

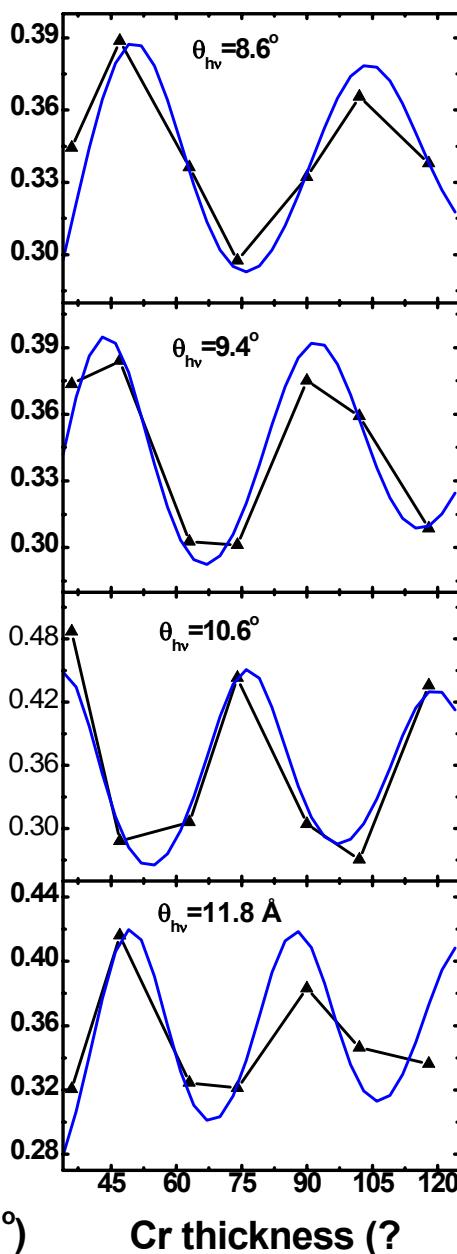
**Sample angle scan
for rocking curve**

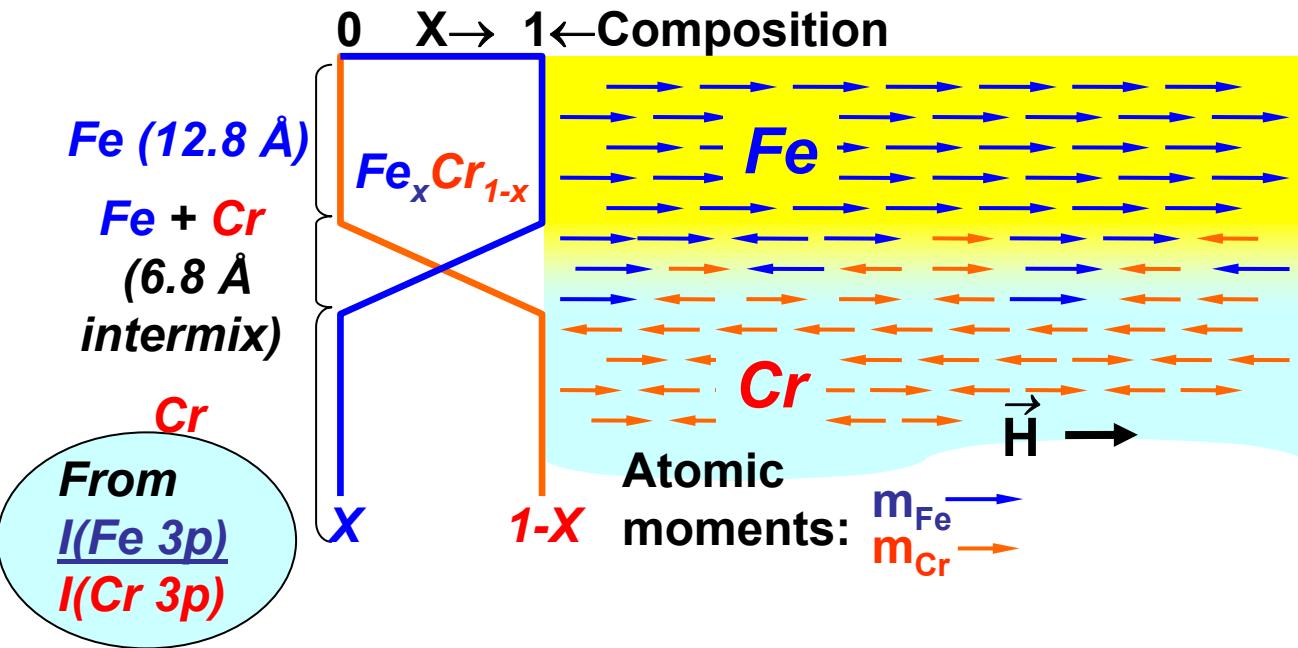


Rocking curves



**Sample scan =
Cr thickness depend.**



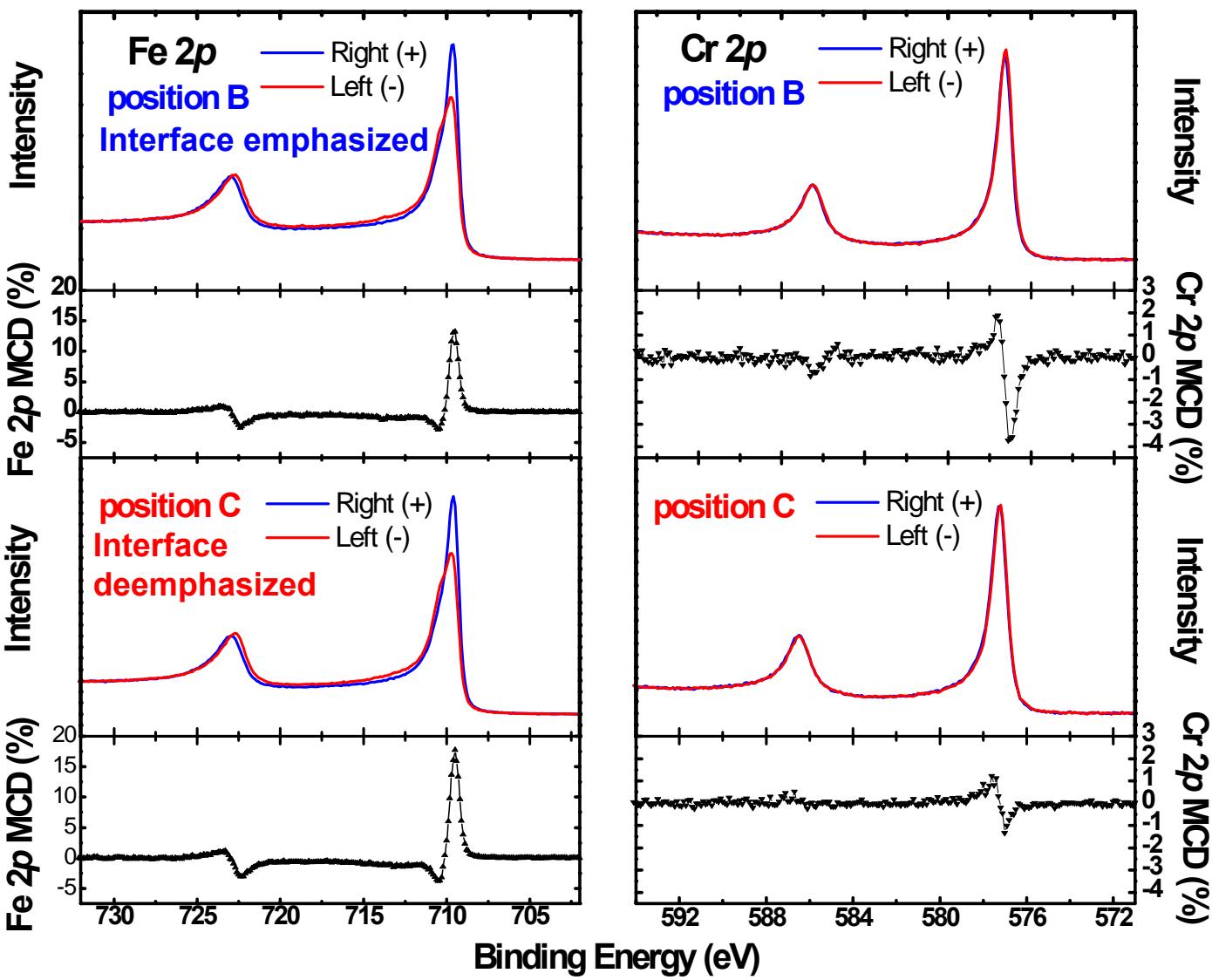
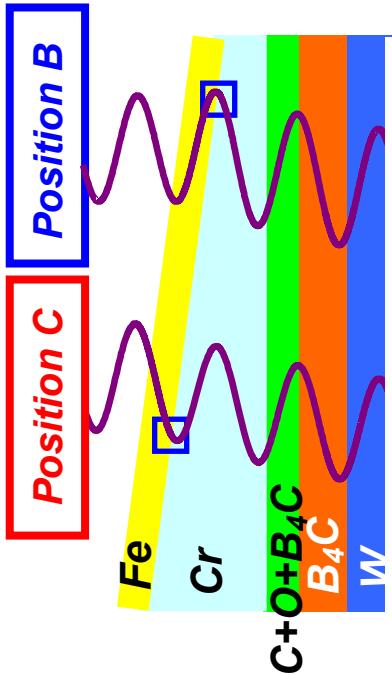


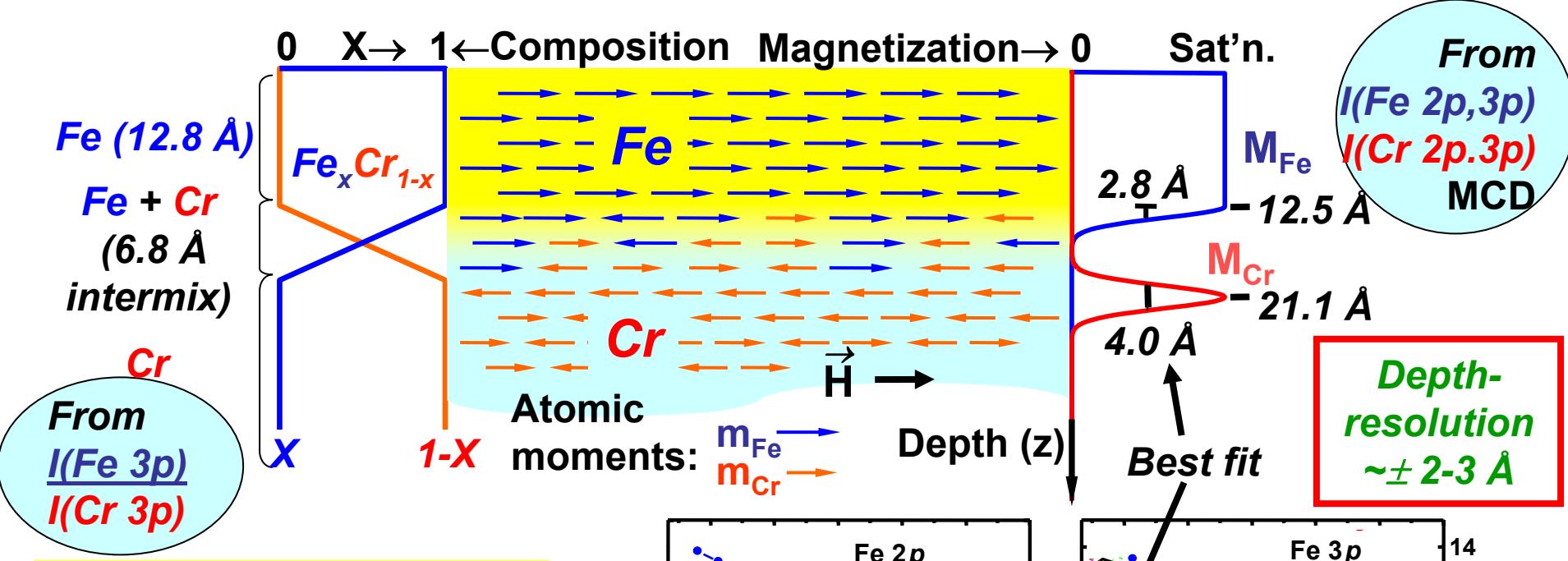
Fitting core PS
 experiment to XRO
 theory: non-
 destructive,
 depth-resolved
 determination of
 composition

Fe and Cr 2p magnetic circular dichroism--probe of y-axis magnetization

Fe and Cr 2p MCD data from Fe/Cr wedge/multilayer

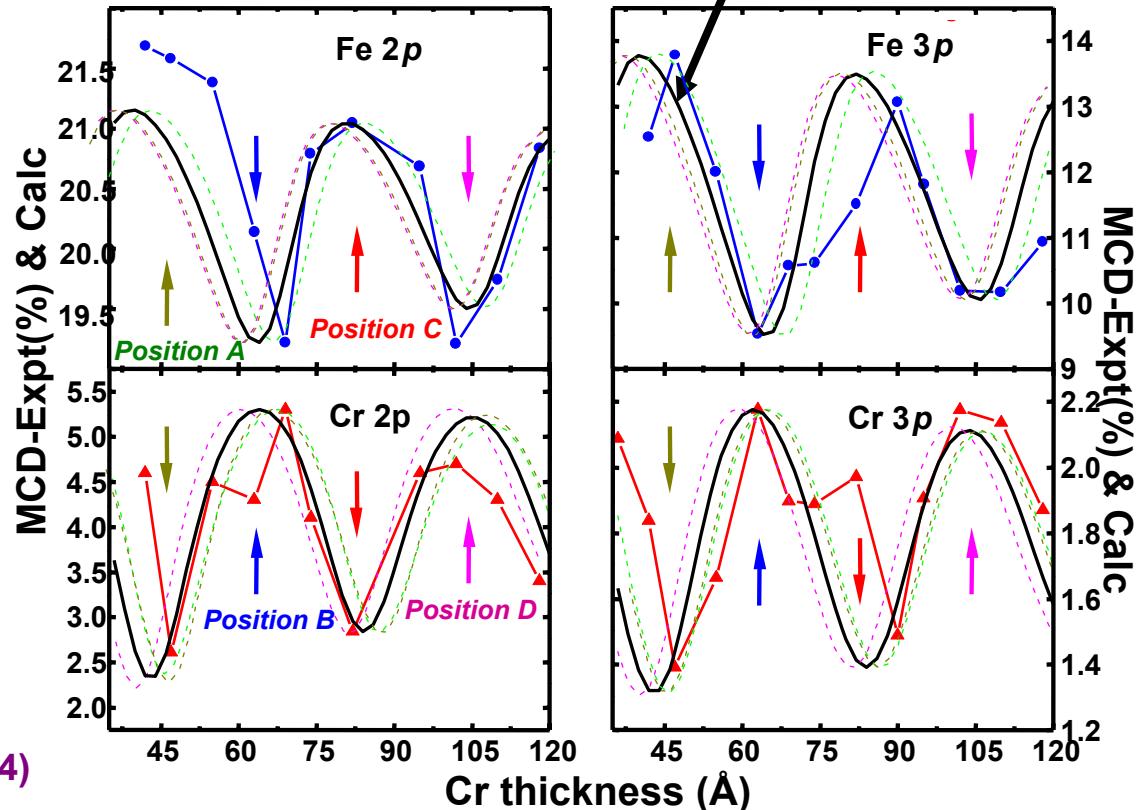
**Cr magnetization
Is antiparallel to
Fe; systematic
variation of MCD
strengths vs d_{cr}**

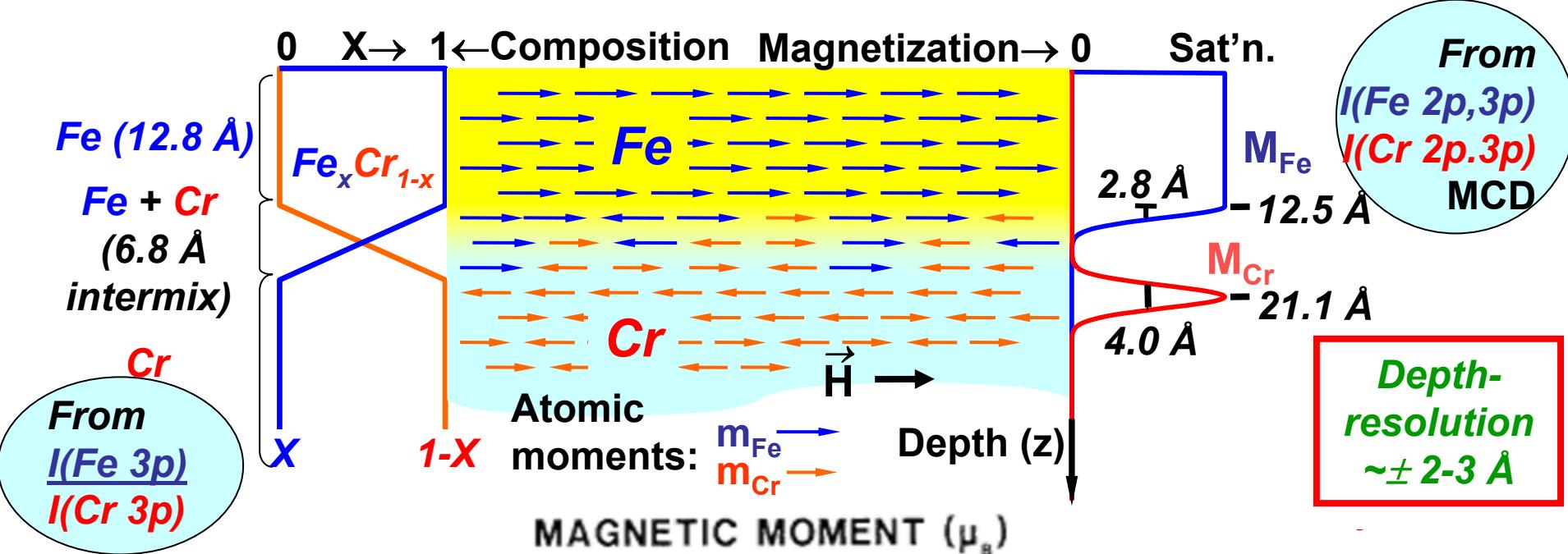




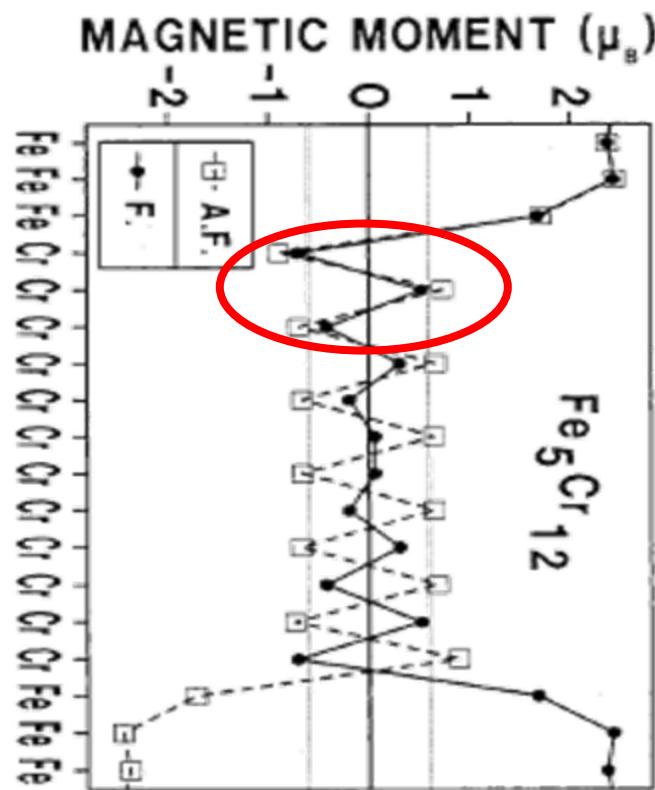
Fitting core PS experiment to XRO theory: non-destructive, depth-resolved determination of composition and magnetization profiles

S.-H. Yang, B.S. Mun et al.,
Surf. Sci. Lett. 461, L557 (2000);
Phys. Cond. Matt. 14, L406 (2002);
Synch. Rad. News 17 (no. 3), 24 (2004)





And what does theory say?



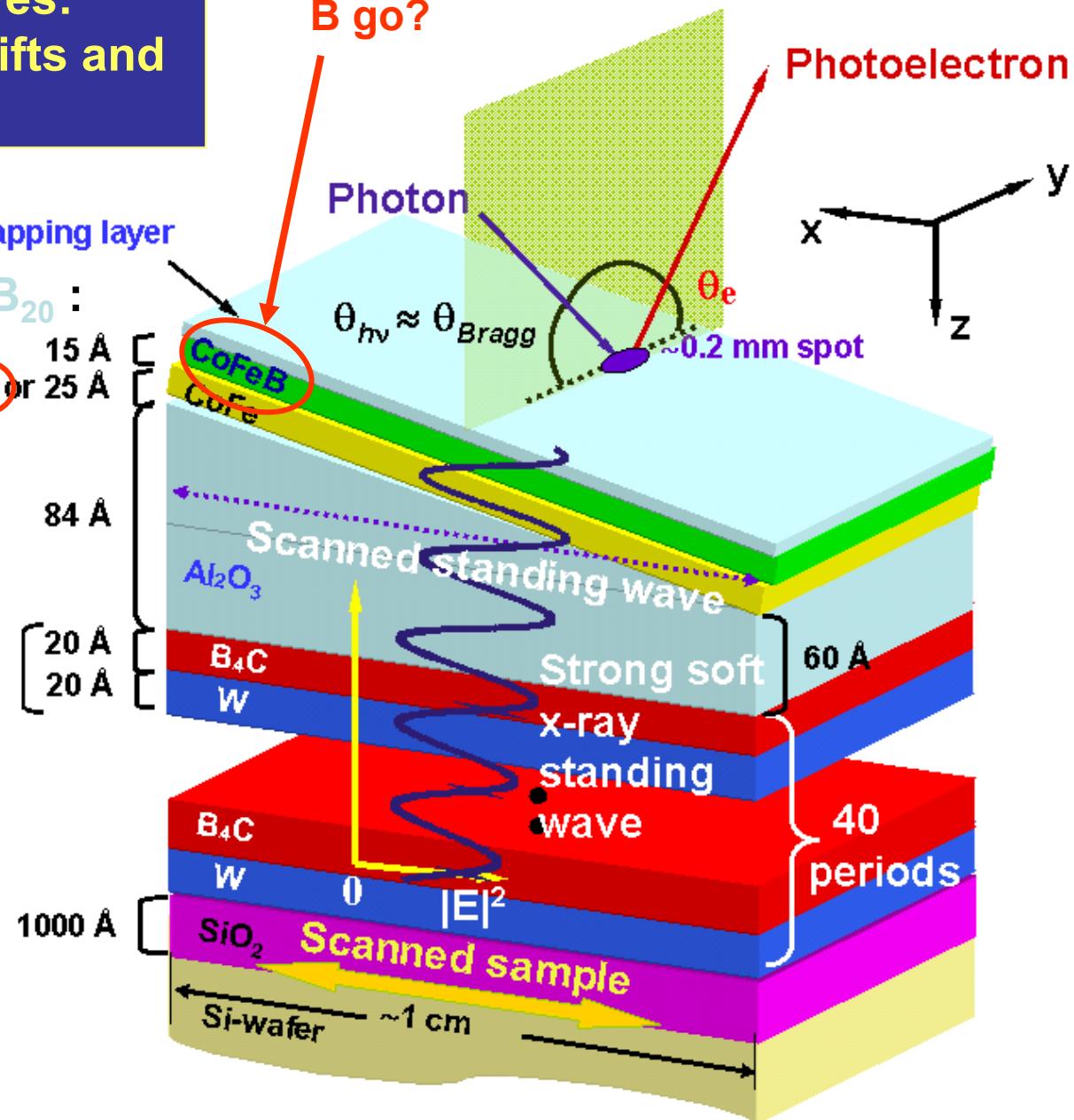
Spin-density wave theory
for an ideal epitaxial interface
(Fishman, J. Phys. Cond. Matt. 13, R235 (2001))

Probing Buried Interfaces with Soft X-ray Standing Waves: Core-Level Chemical Shifts and Valence Band DOSs

$\text{Al}_2\text{O}_3/\text{Co}_{70}\text{Fe}_{30}/\text{Co}_{56}\text{Fe}_{24}\text{B}_{20}$:
model system for
magnetic tunnel
resistance

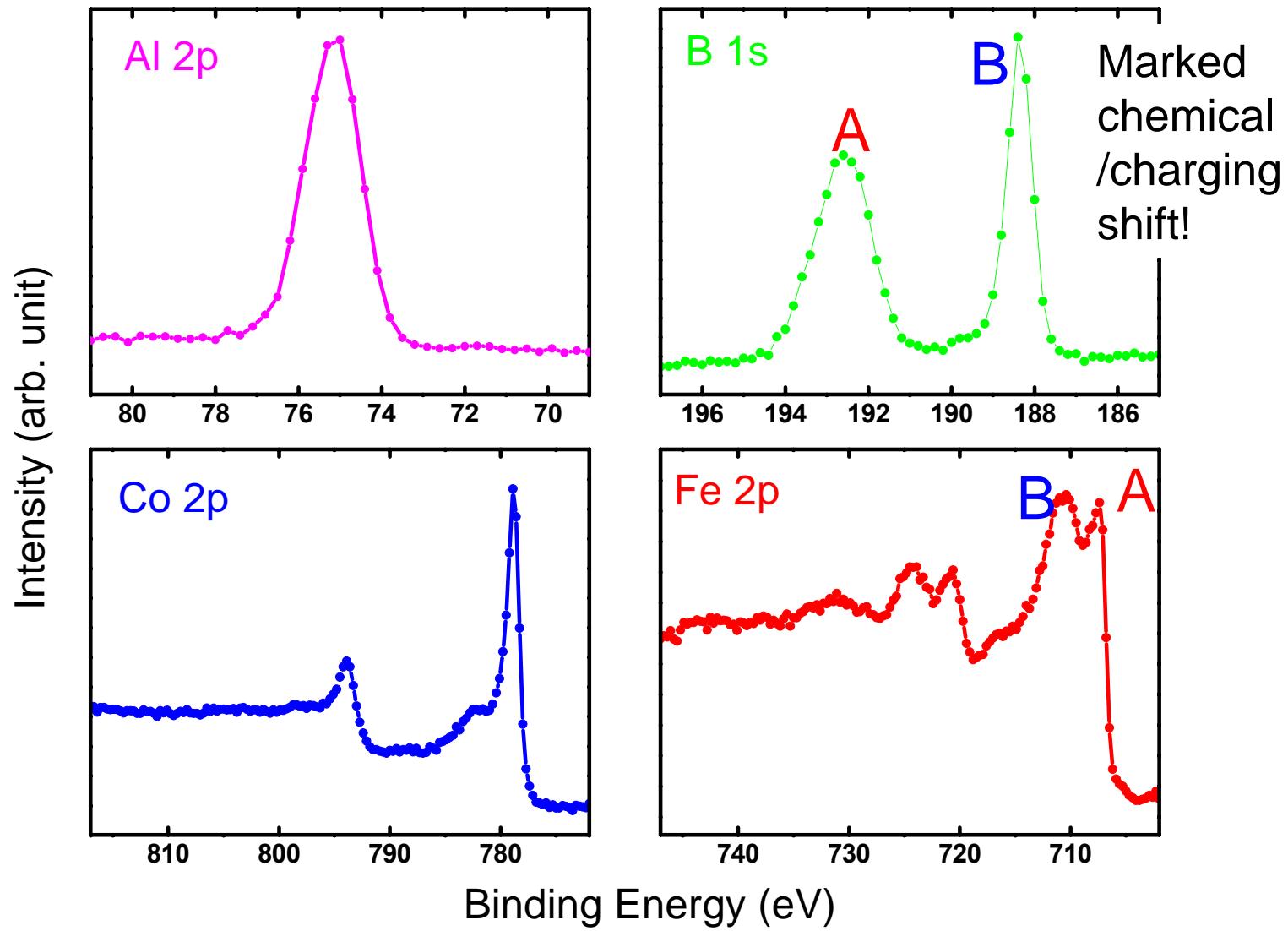
Higher Tunnel
Resistance
(45% \rightarrow 65%),
Lower coercive
fields
(45 Oe \rightarrow 5 Oe)—
Why?

Where does the
B go?



With S.-H. Yang,
S. Parkin. IBM

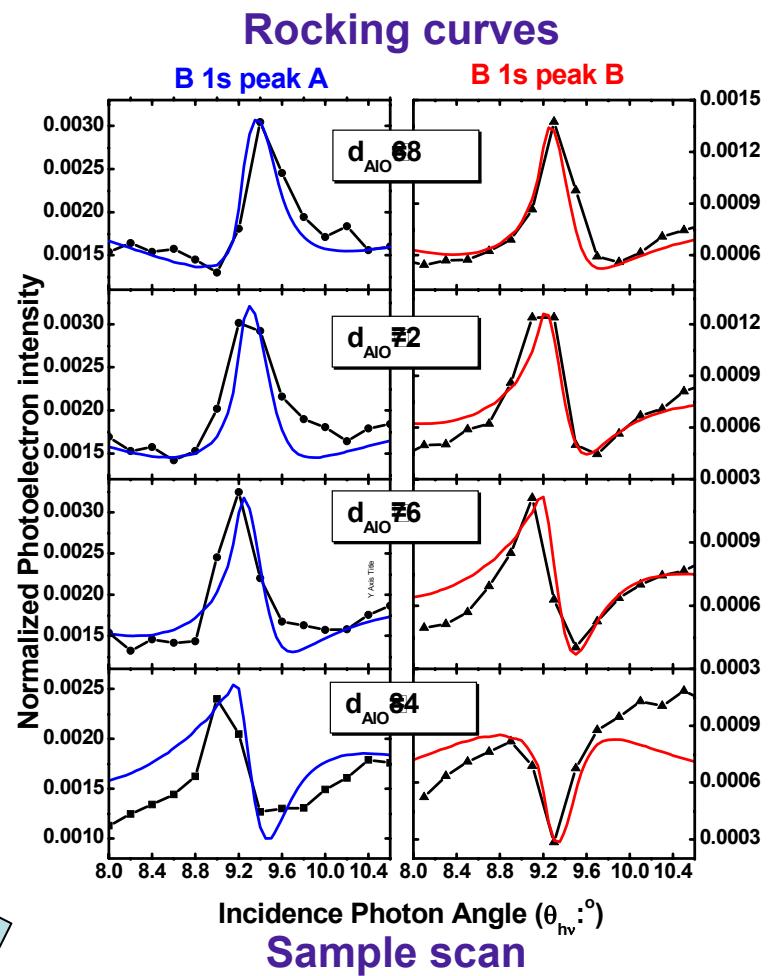
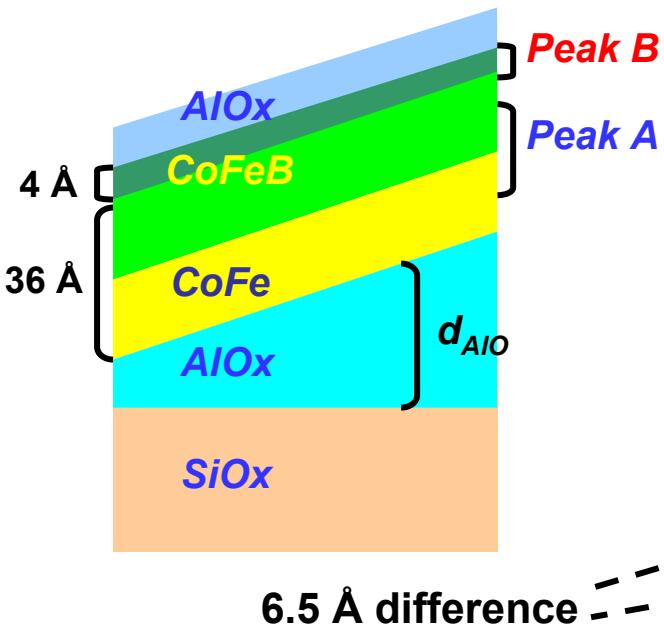
Core-level photoemission spectra



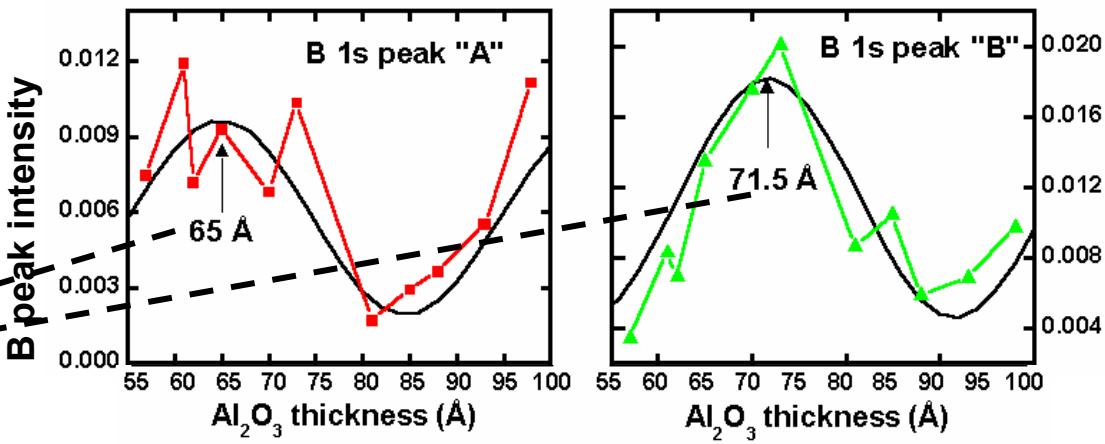
Rocking curve and sample scan analysis: B 1s data

*Peak A : B 1s from
CoFeB amorphous
layer + CoFe alloy*

*Peak B : B 1s from
topmost CoFeB layers*

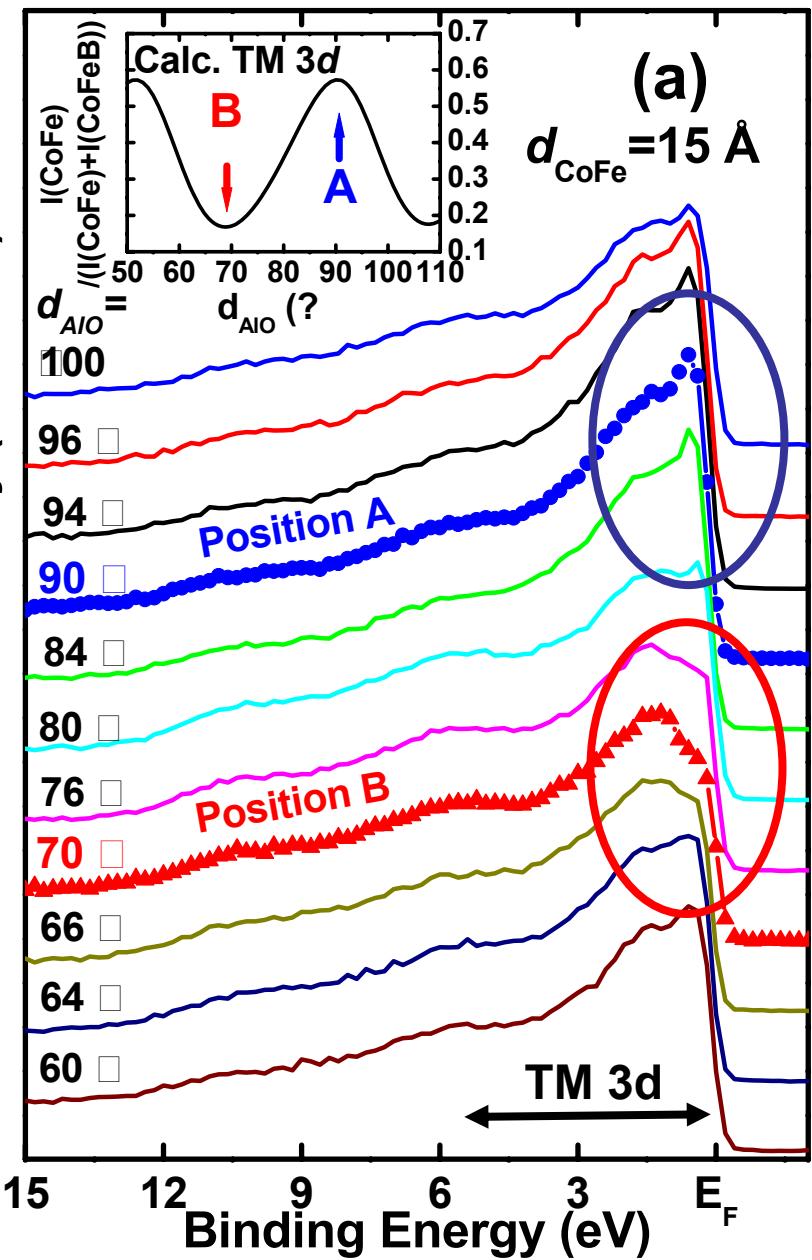


Sample scan

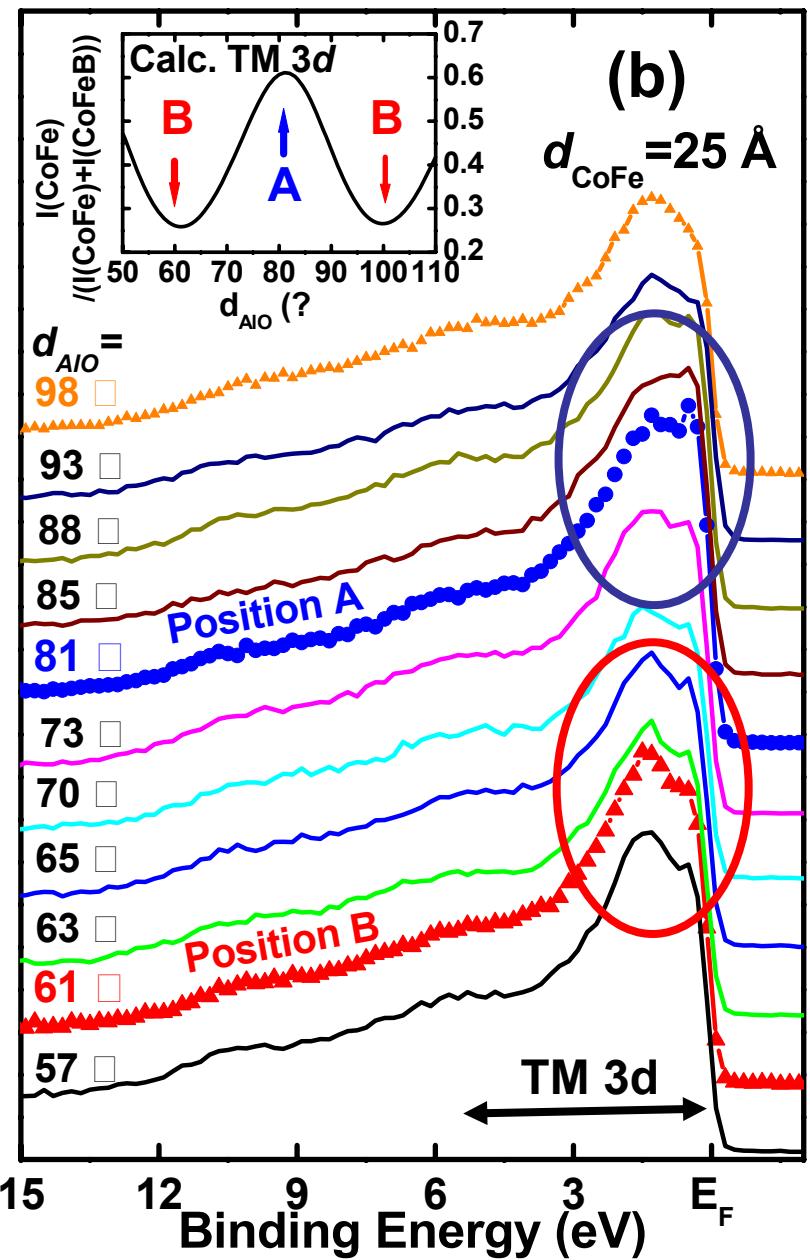


Valence-band spectra as a function of standing wave position

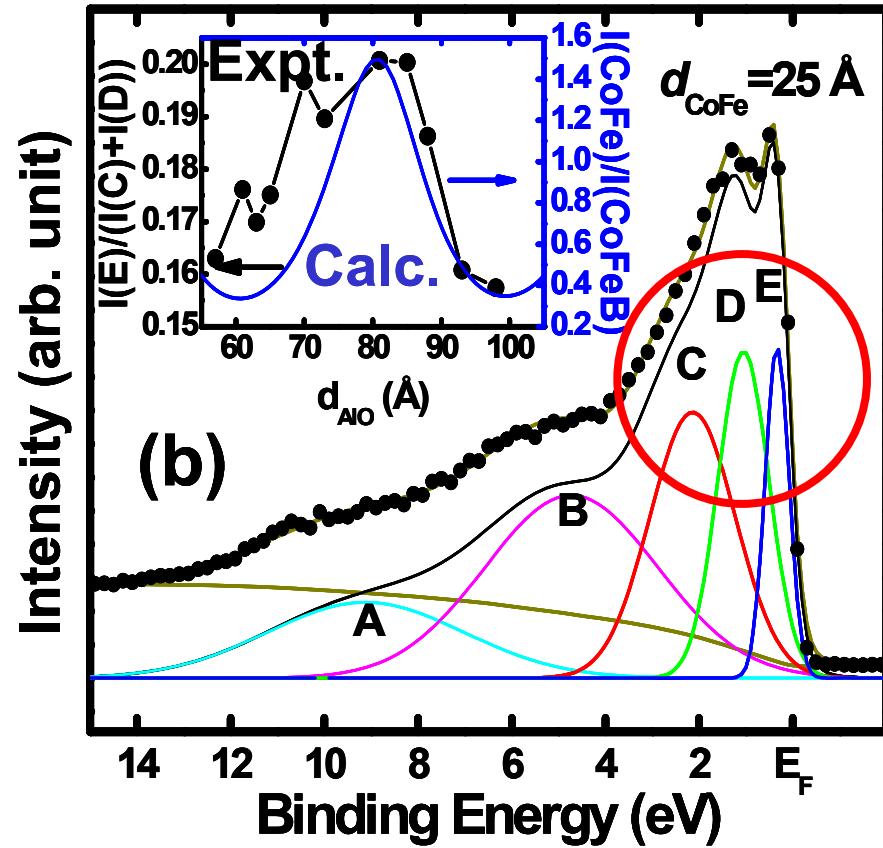
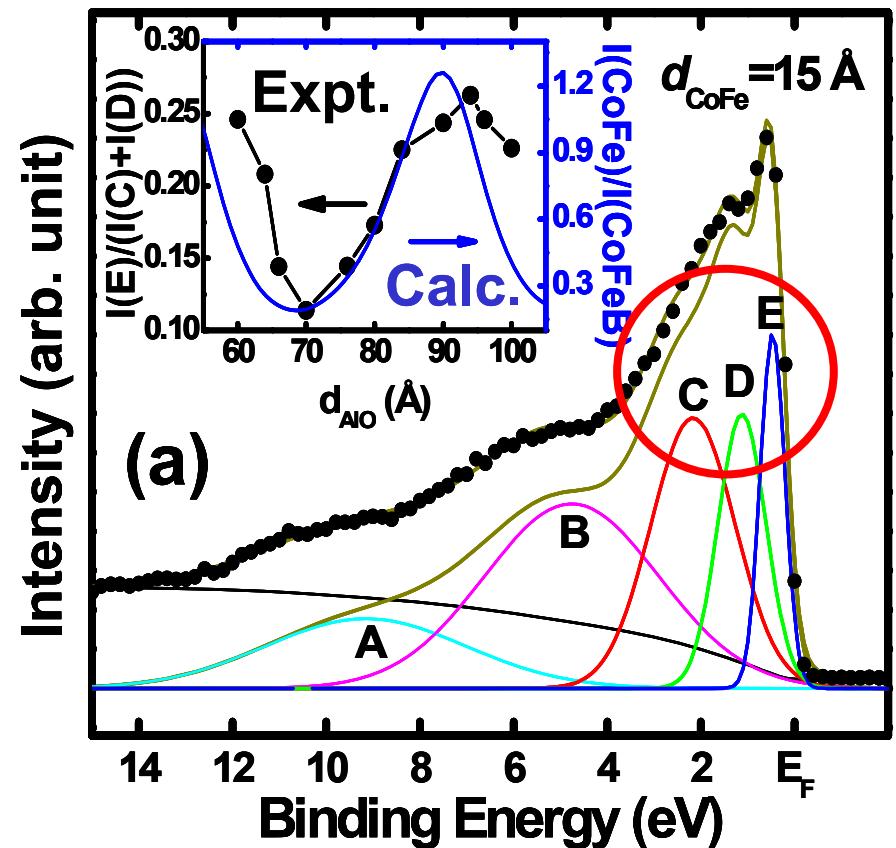
Valence-Band Intensity (arb. unit)



Valence-Band Intensity (arb. unit)



Extraction of depth-resolved densities of states in FM layers



Measure $R^{E,C} = I_E/I_C$ and $R^{D,C} = I_D/I_C$
as fn. of standing wave position,
Use with x-ray optical theory to
deconvolve layer-by-layer
contributions

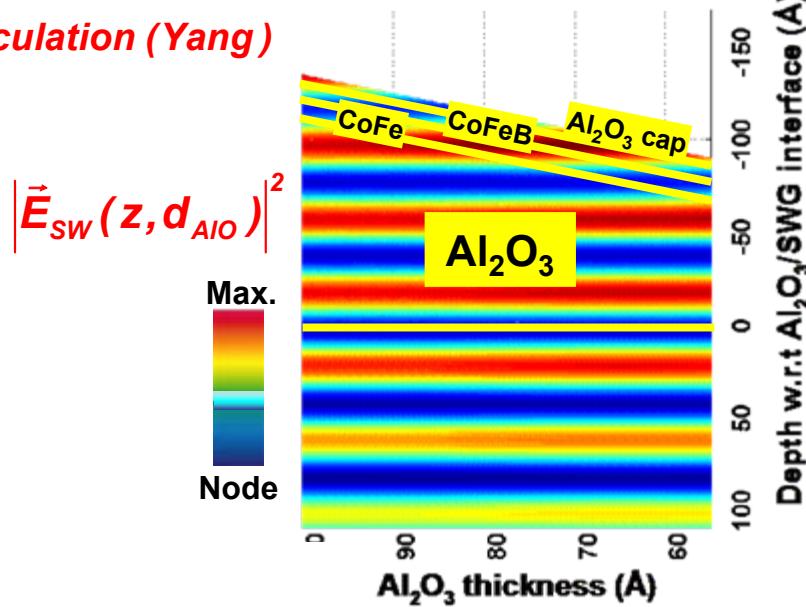
Deconvolving layer densities of states from standing wave data

With $i = \text{Co}_{56}\text{Fe}_{24}\text{B}_{20}, \text{Co}_{70}\text{Fe}_{30}$: $R_{(0)i}^{D,C} = I_{(0)i}^D / I_{(0)i}^C; R_{(0)i}^{E,C} = I_{(0)i}^E / I_{(0)i}^C$ assumed constant within each layer

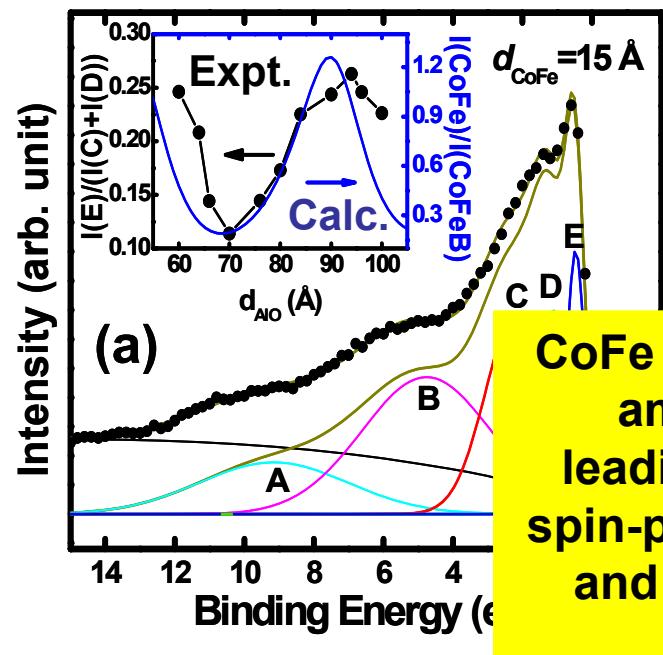
With $j = D, E$:

$$I_i^j(d_{AIO}) = CR_{(0)i}^{j,C} \int_{\Delta z(i) = \text{layer thickness}} |\vec{E}_{SW}(z, d_{AIO})|^2 [\rho_{Co,i} \frac{d\sigma_{Co3d}}{d\Omega} + \rho_{Fe,i} \frac{d\sigma_{Fe3d}}{d\Omega}] \exp[-z / (\Lambda_e(E_{kin}^j) \sin \theta)] dz$$

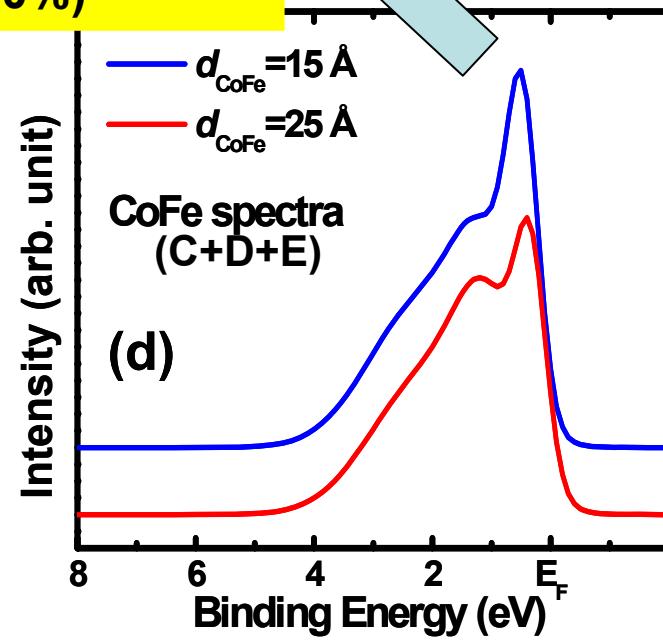
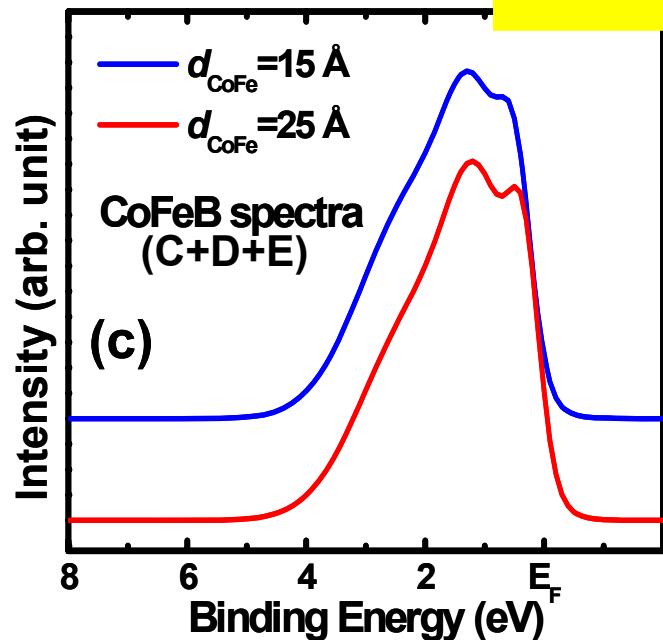
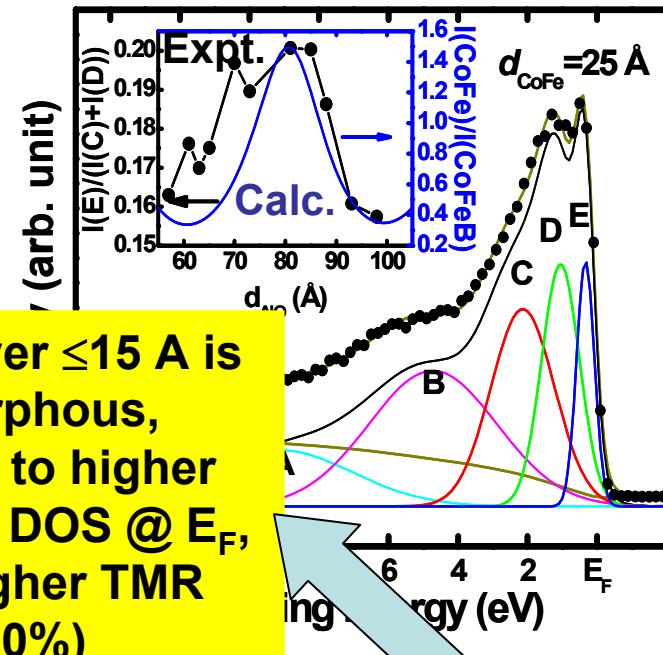
$= CR_{(0)i}^{j,C} \beta_i(d_{AIO})$; $\beta_i(d_{AIO})$ from x-ray optical calculation (Yang)



Extraction of depth-resolved densities of states in FM layers

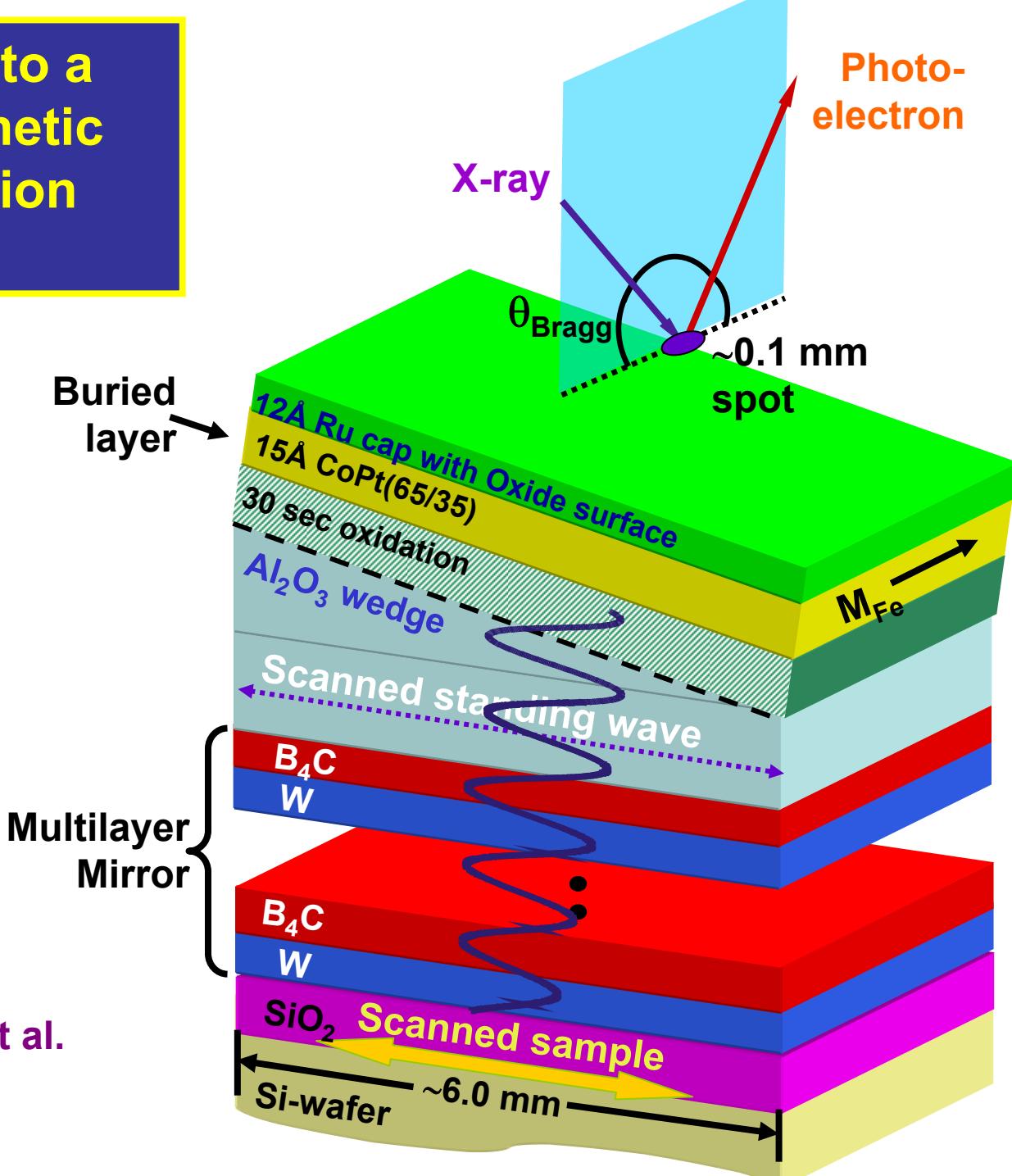


CoFe layer $\leq 15 \text{ \AA}$ is amorphous, leading to higher spin-pol. DOS @ E_F , and higher TMR (60%)



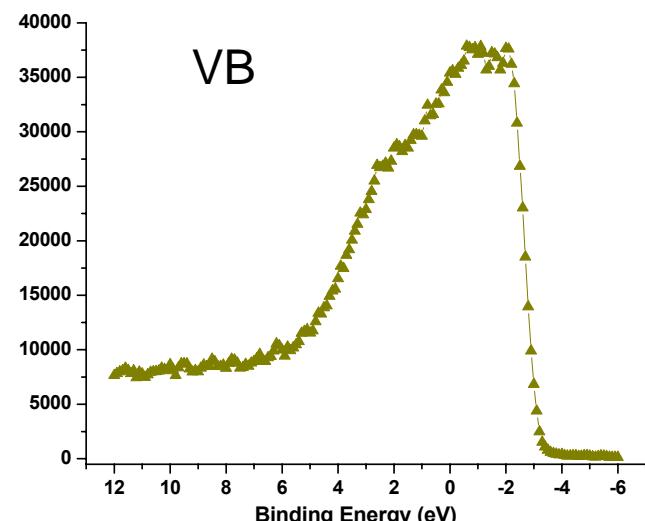
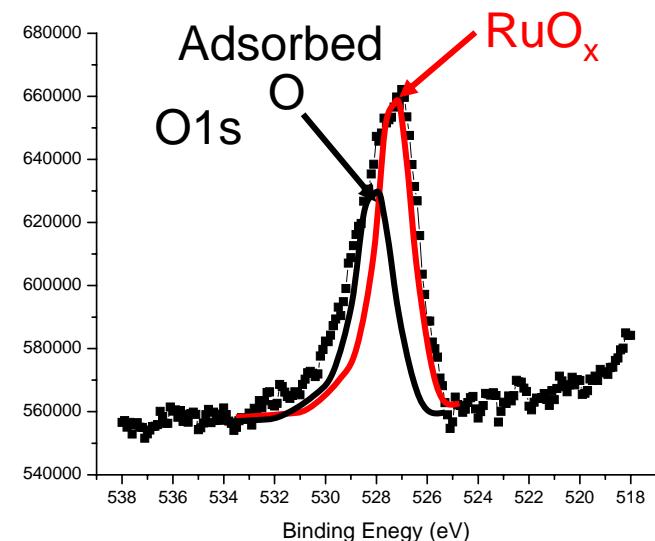
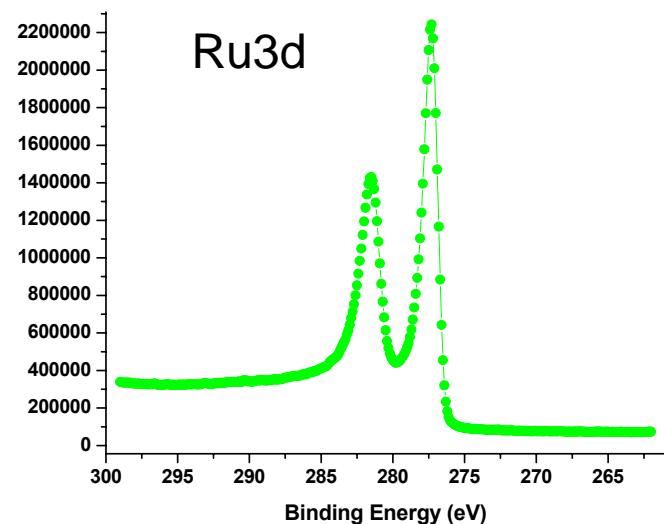
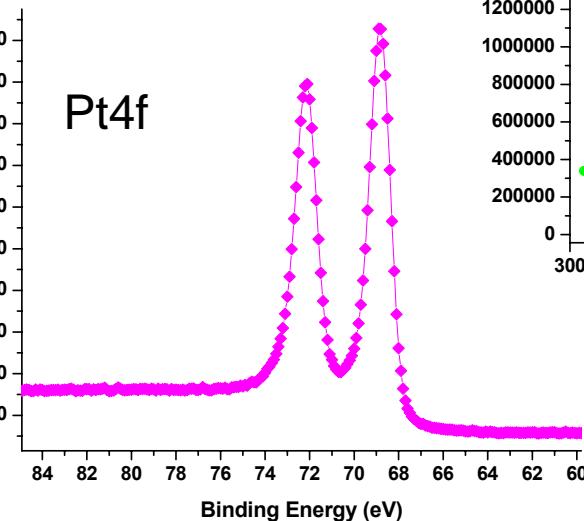
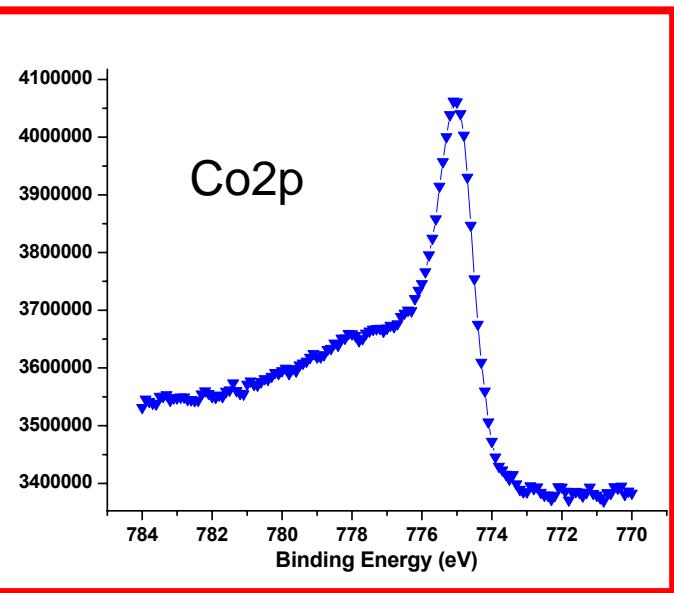
Deconvoluted CoFeB and CoFe DOSs

Application to a second magnetic tunnel junction system

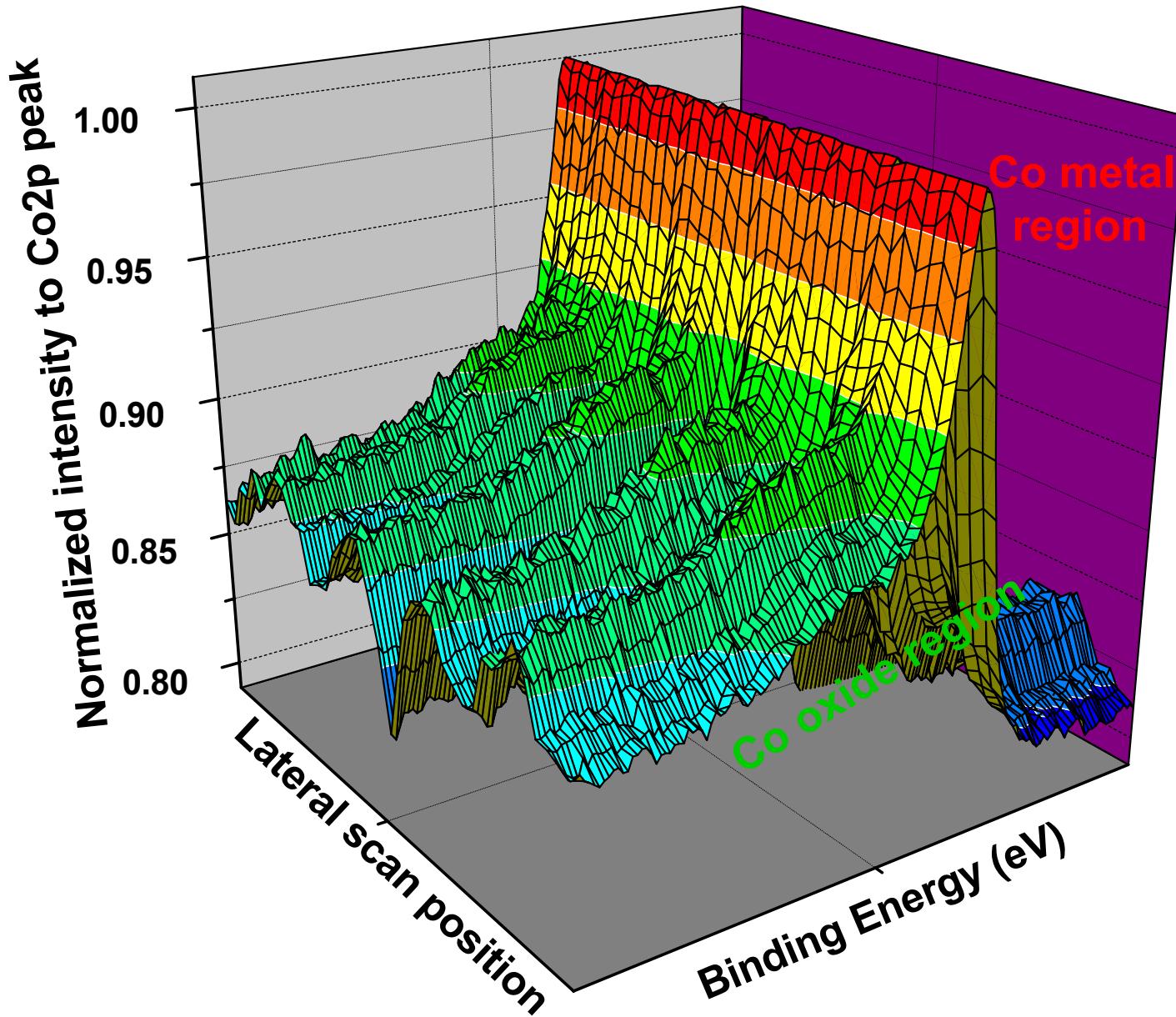


Sell, Yang, Parkin et al.

Representative spectra:



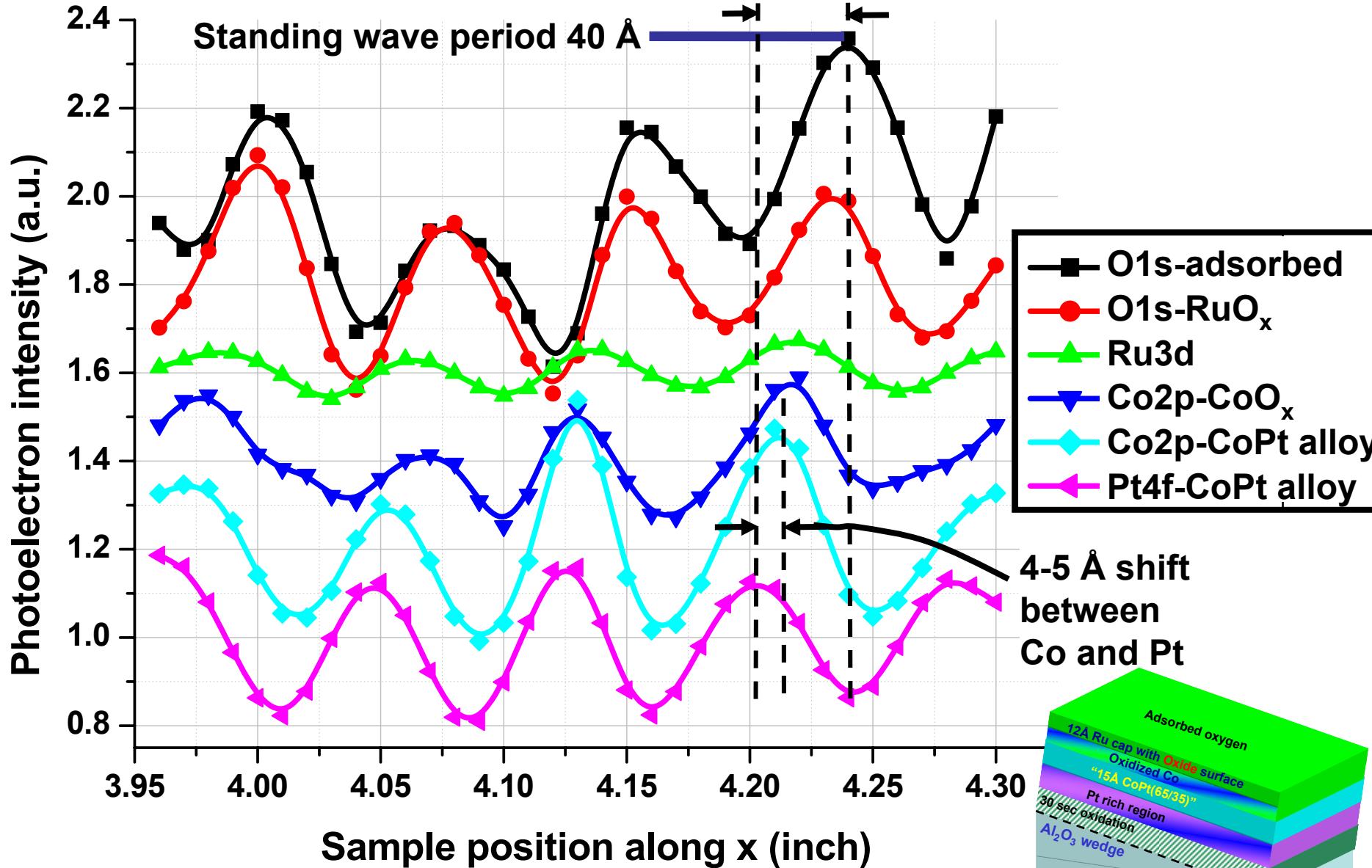
Co 2p spectrum during a standing wave scan

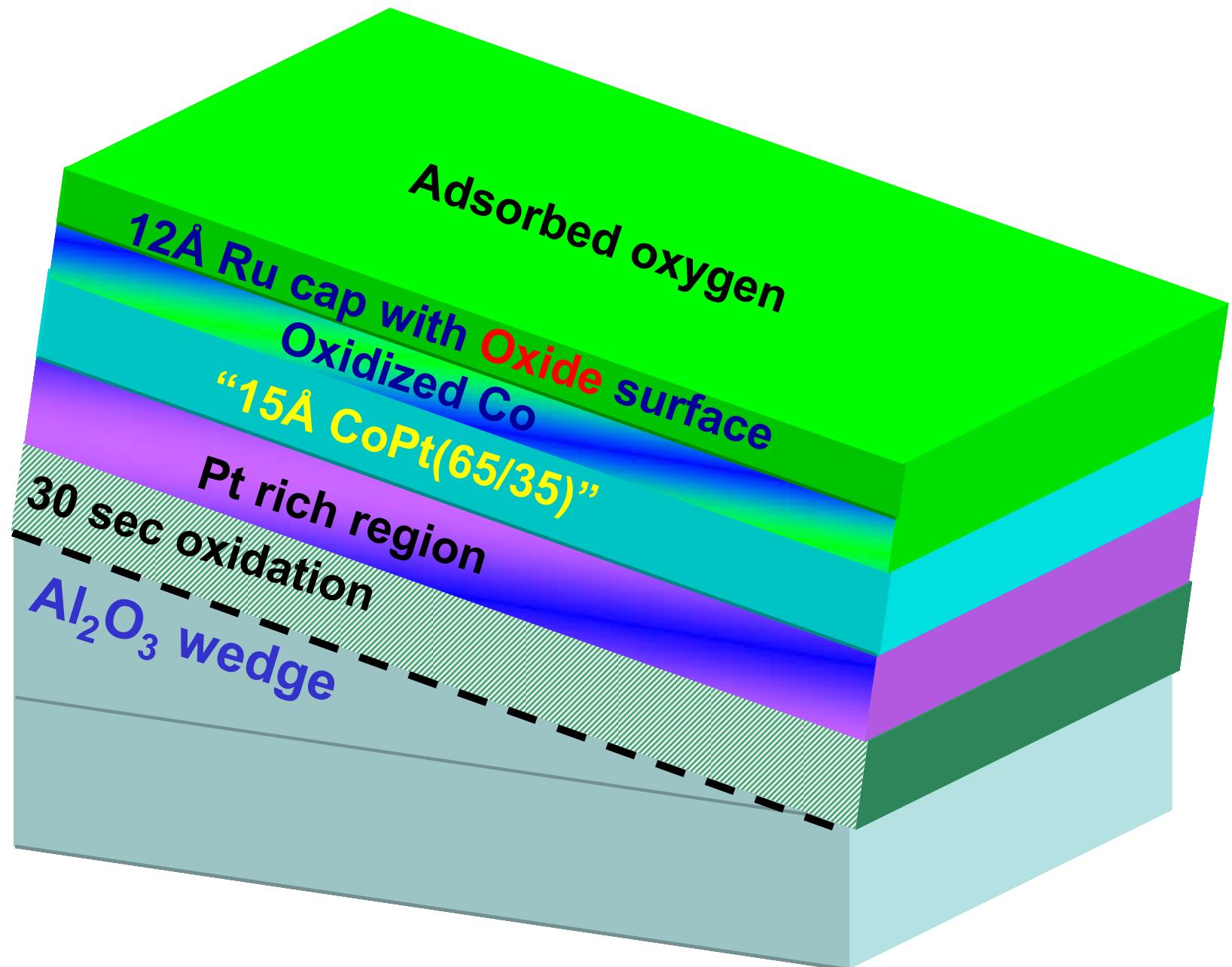


"Average depths with a ruler"

Deeper ← Surface

18.6 Å

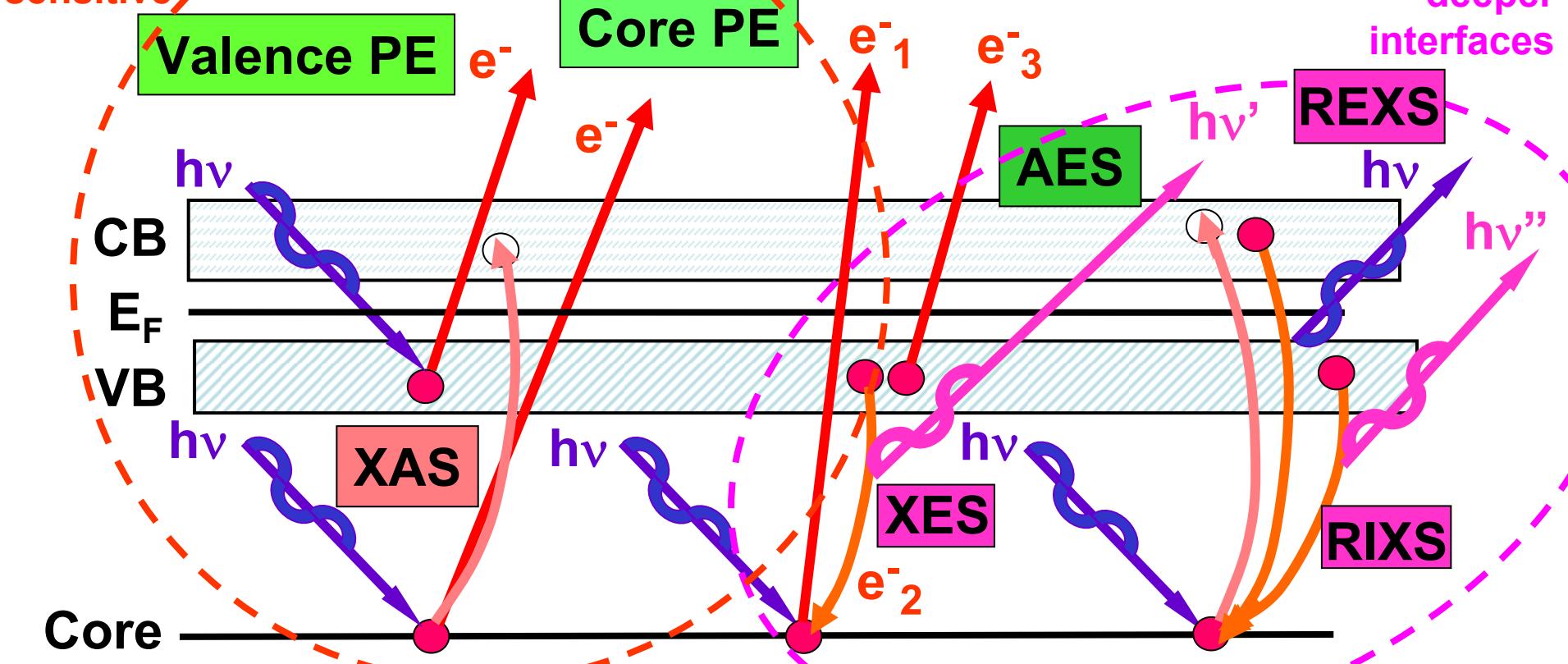




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- Photon-in/electron-out studies of spintronic nanolayer structures
- Photon-in/photon-out studies of spintronic nanolayer structures—some first results
- Future possibilities with photon-in/photon-out, including gas-solid and liquid-solid interfaces
- Resonant elastic soft x-ray scattering from nanostructures: Toward soft x-ray photonics?

The Soft X-Ray Spectroscopies



PE = photoemission = photoelectron spectroscopy

XAS = x-ray absorption spectroscopy

AES = Auger electron spectroscopy

XES = x-ray emission spectroscopy

REXS/RIXS = resonant elastic/inelastic x-ray scattering

- $n(h\nu) =$

$$1 - \delta(h\nu) + i\beta(h\nu)$$

- variable polarization

- multiple reflection/refraction

- exact treatment of interlayer intermixing a/o roughness

- electric field at i -th layer:

$$|E_{sw,i}(z)|^2 = |E_i^+(z) + E_i^-(z)|^2$$

Photoemission:

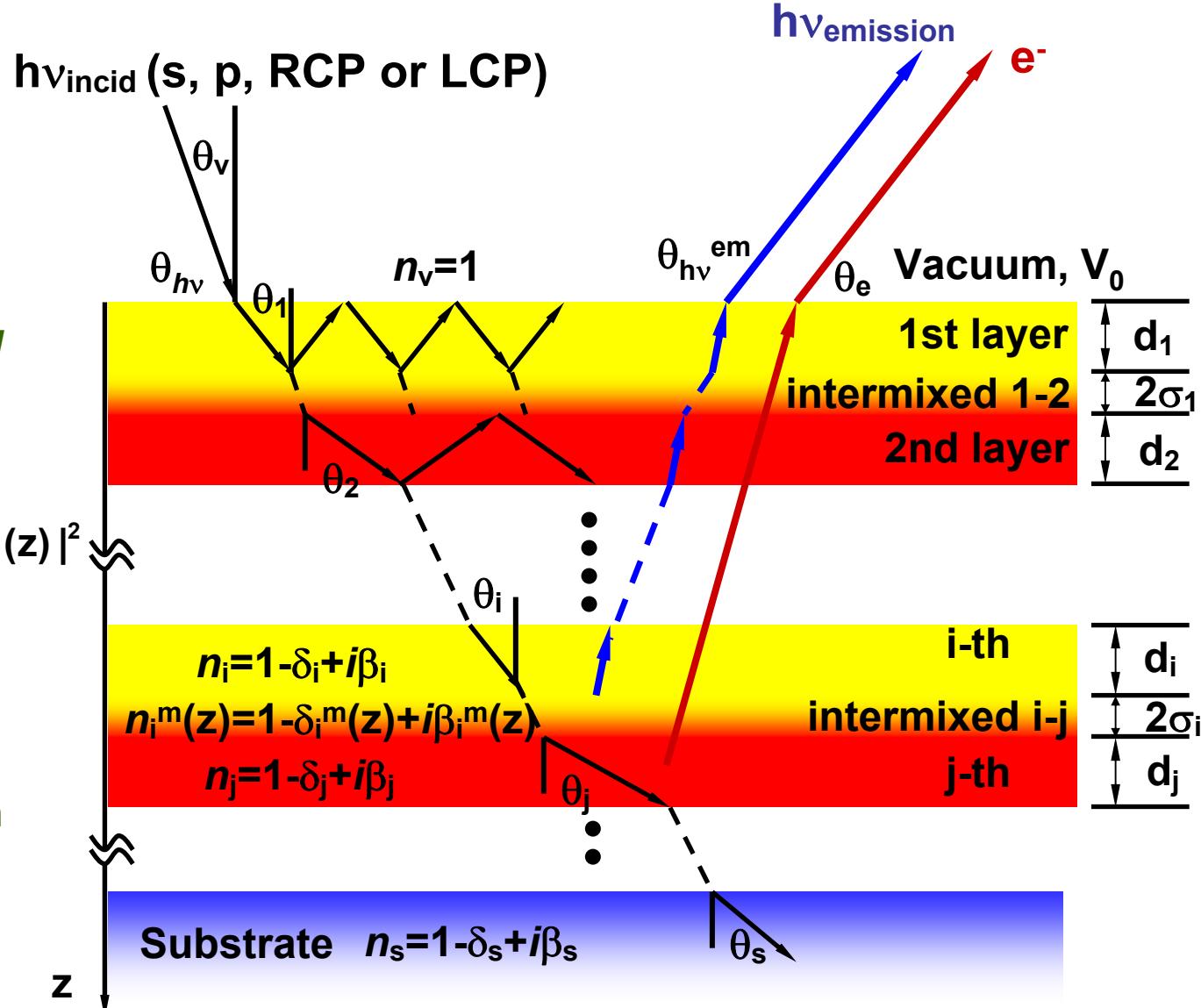
- differential cross section

- inelastic attenuation

- surface refraction

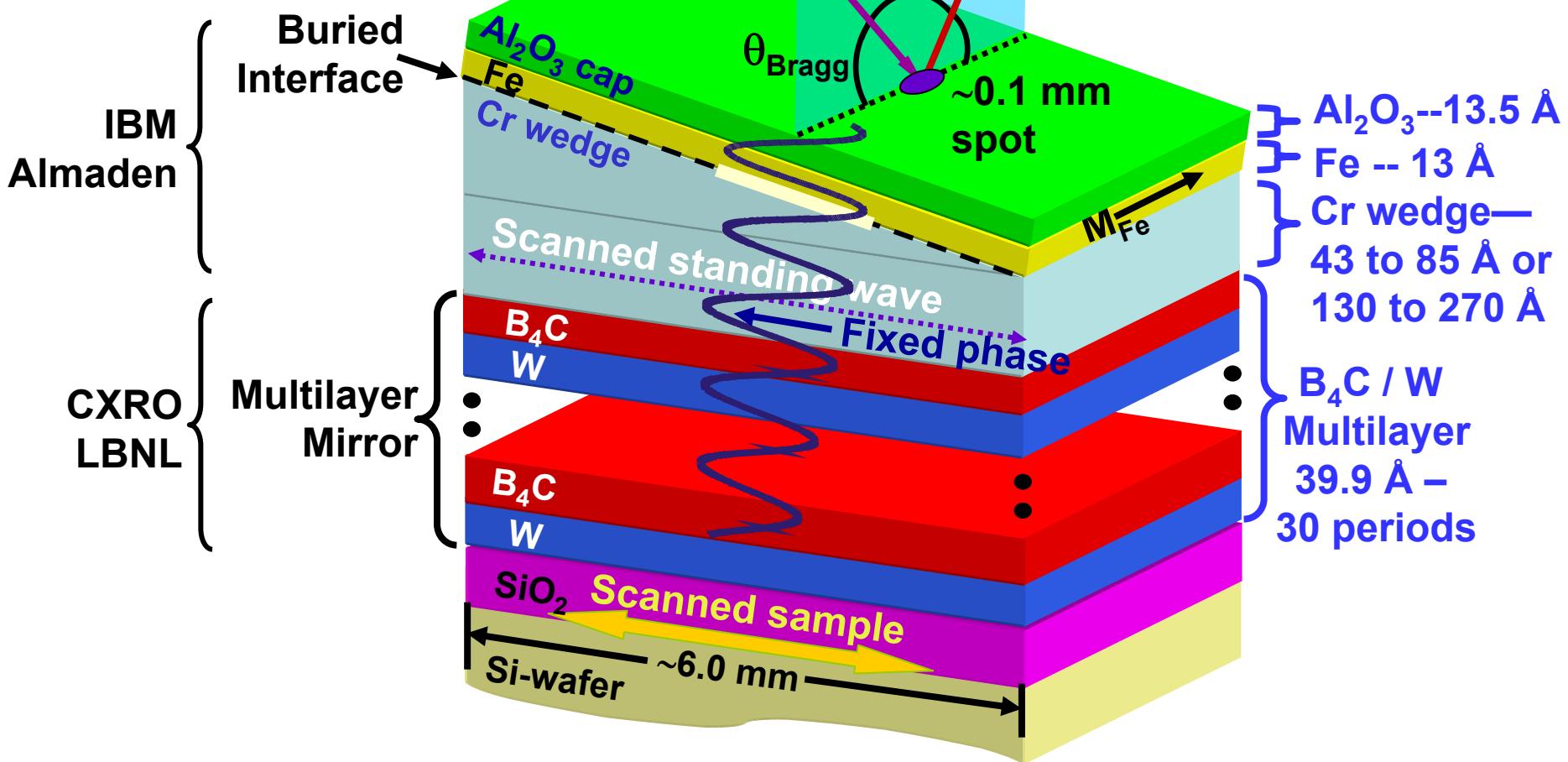
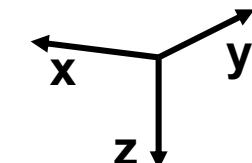
X-ray emission:

- fluorescence yield

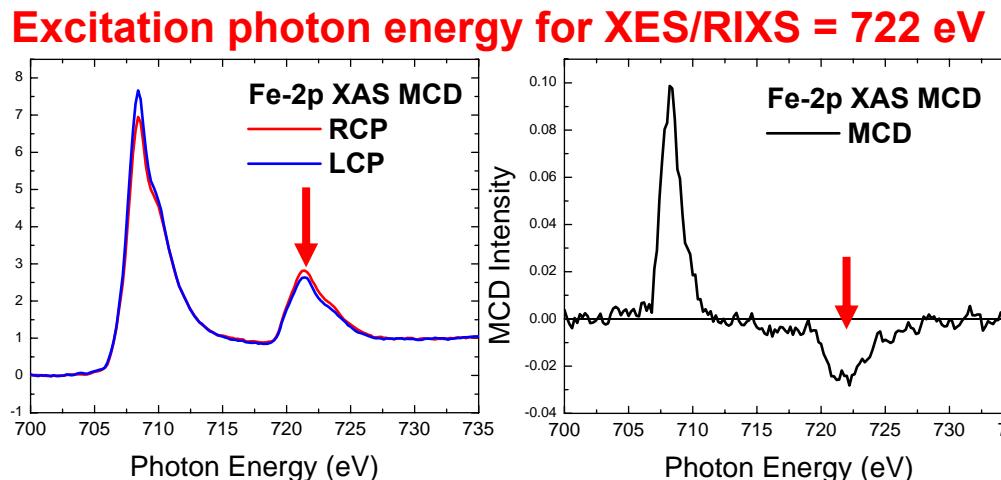
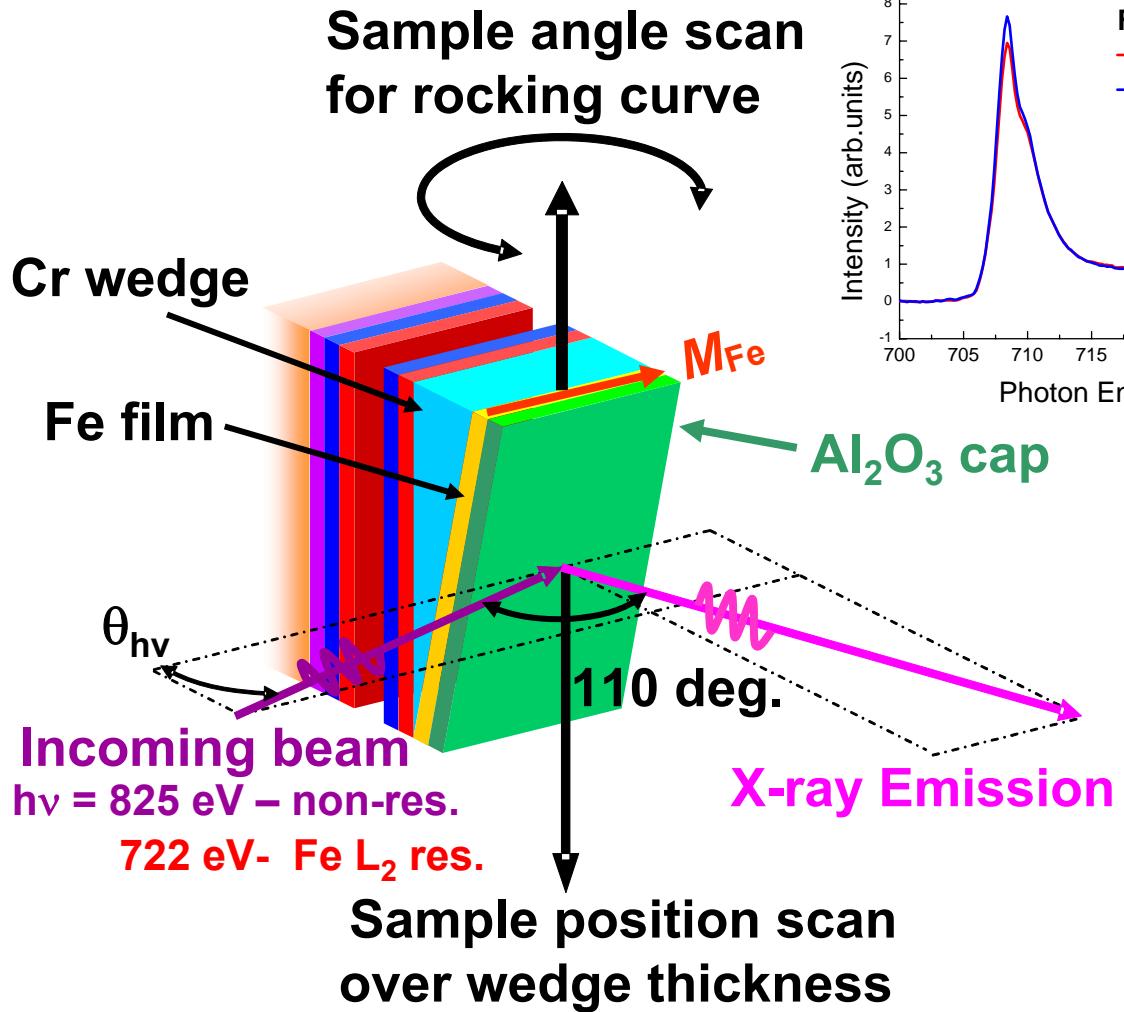


The Standing Wave-Wedge Method

Photon-out:
XES/RIXS
Fe/Cr bilayer
with Al_2O_3 cap



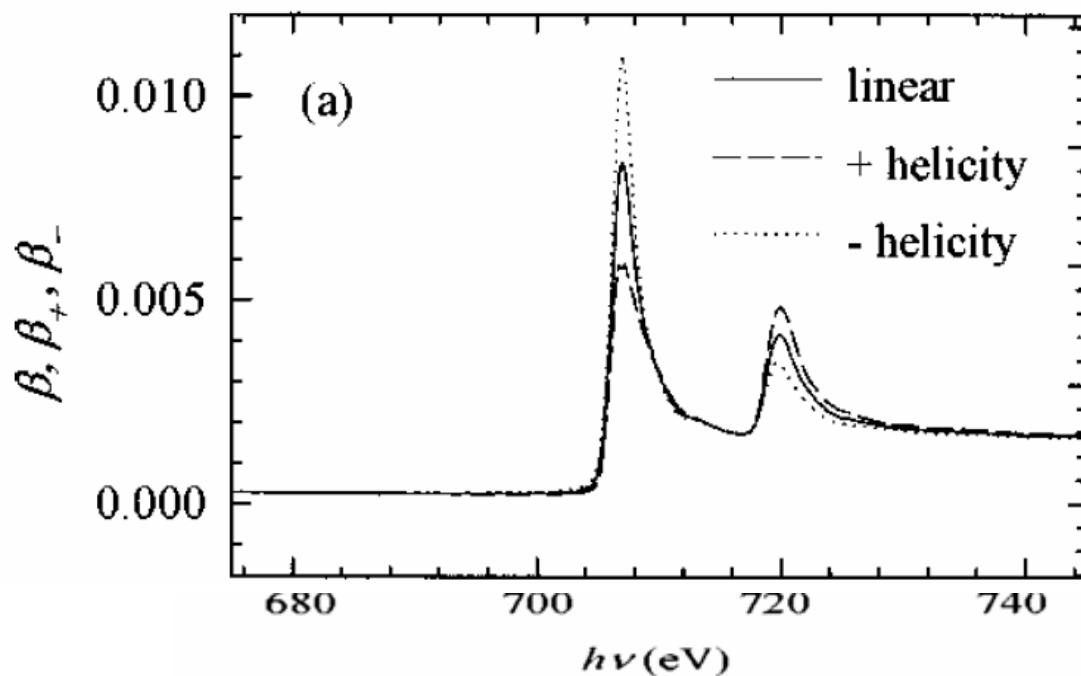
Standing wave excitation of x-ray emission/RIXS in a multilayer magnetic structure



**Reference data: Fe 2p MCD in XAS:
Al₂O₃(cap) / Fe / Cr / B₄C-W SWG**

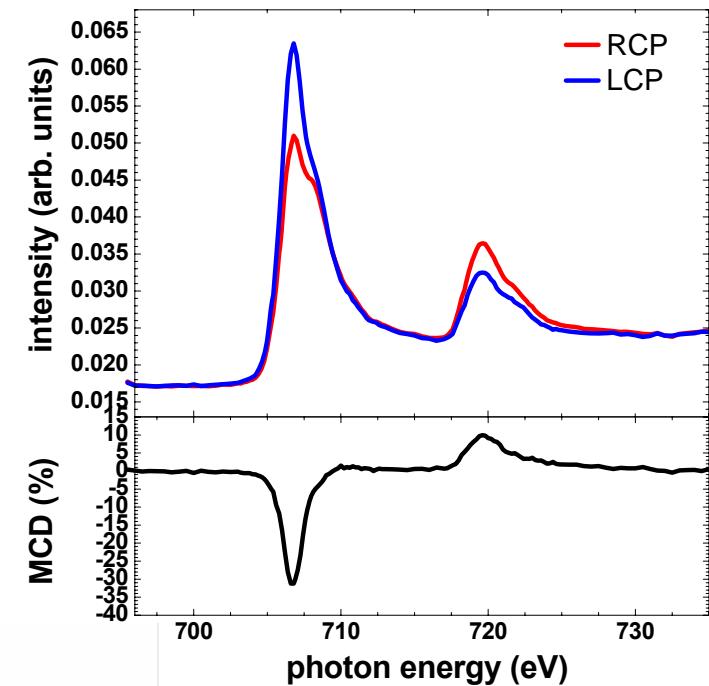
Bulk Fe

MCD = **64%**



Fe in multilayer

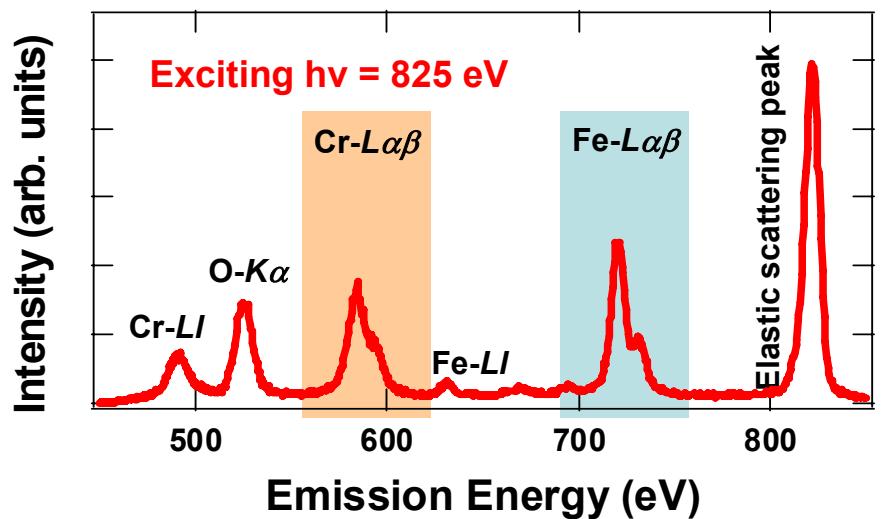
MCD = **32%**



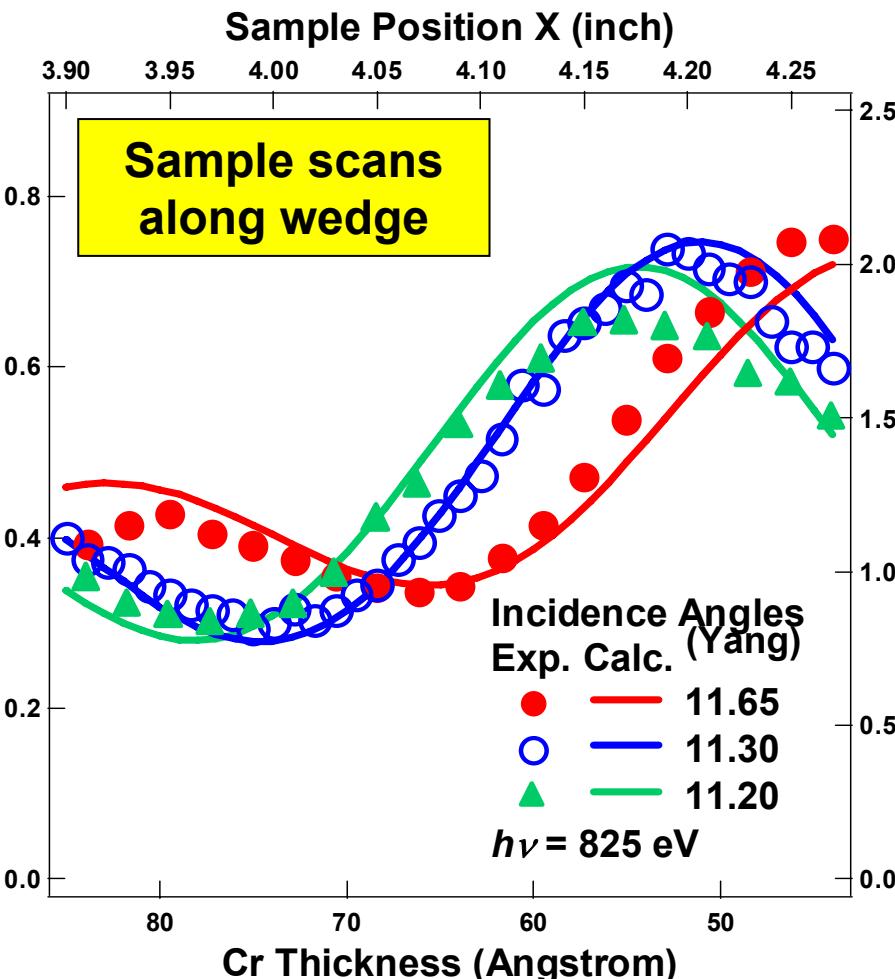
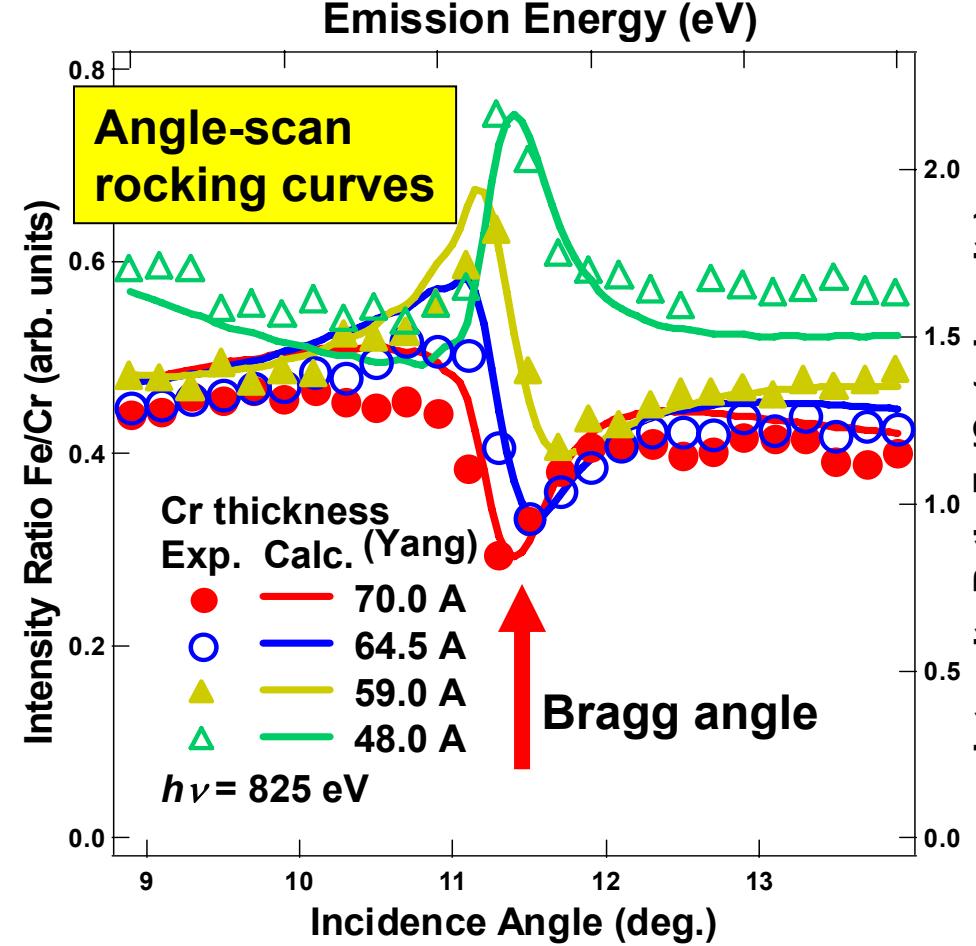
PRB 62, 12216 (2000), Fig. 4,
J.B. Kortright and S.-K. Kim



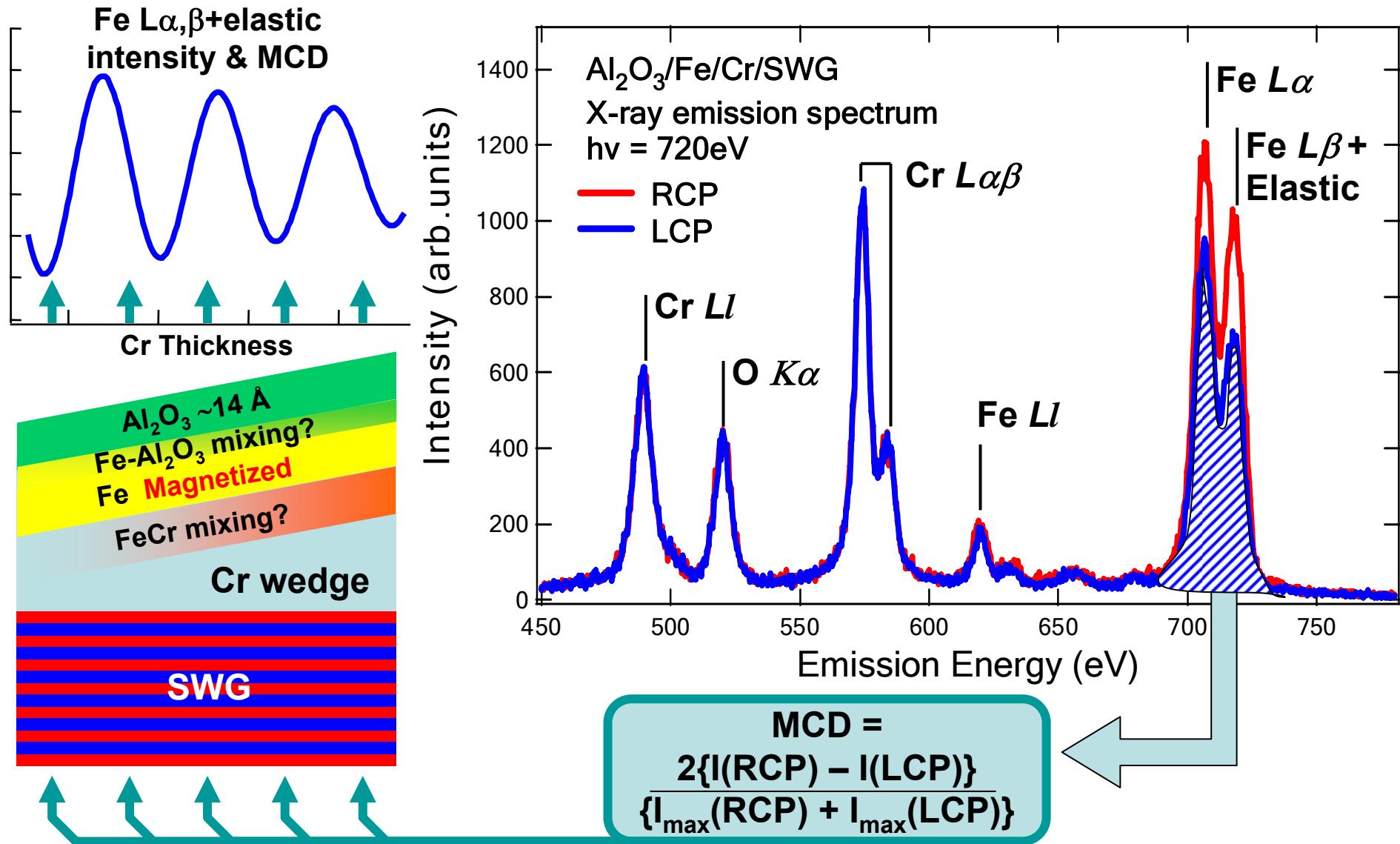
Is roughly half of the Fe layer non-magnetic?



**Experimental + Calculated
X-Ray Emission Intensity Ratio
 $I(\text{Fe } L\alpha\beta)/I(\text{Cr } L\alpha\beta)$ from Fe/Cr wedge
on multilayer mirror**

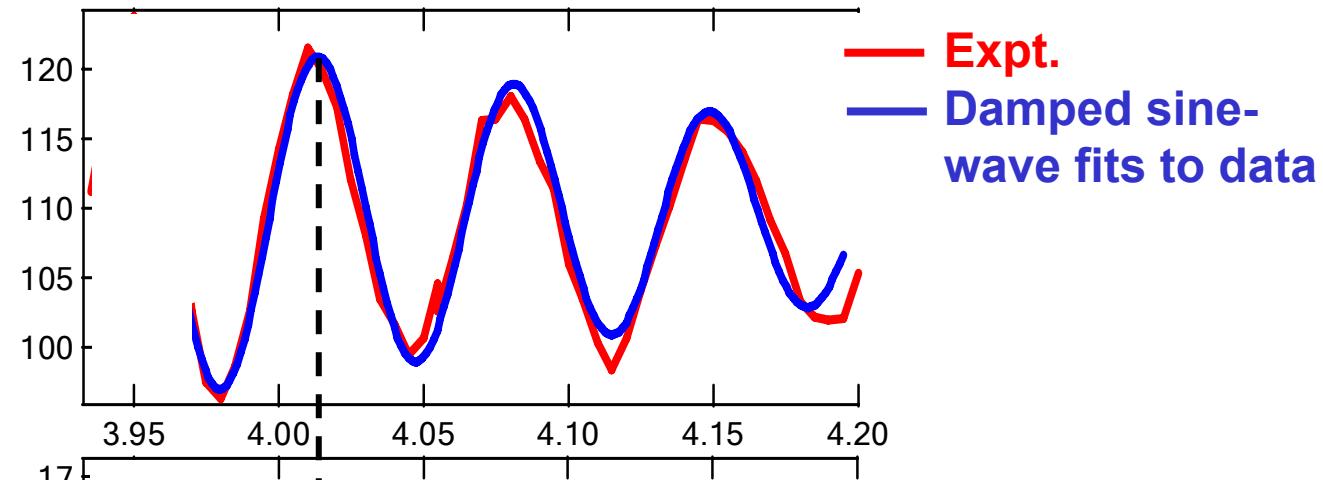


Typical RIXS spectra for MCD measurement
 $h\nu = 720\text{eV}$: Al_2O_3 13Å / Fe 16.2Å / Cr 126-238Å / SWG

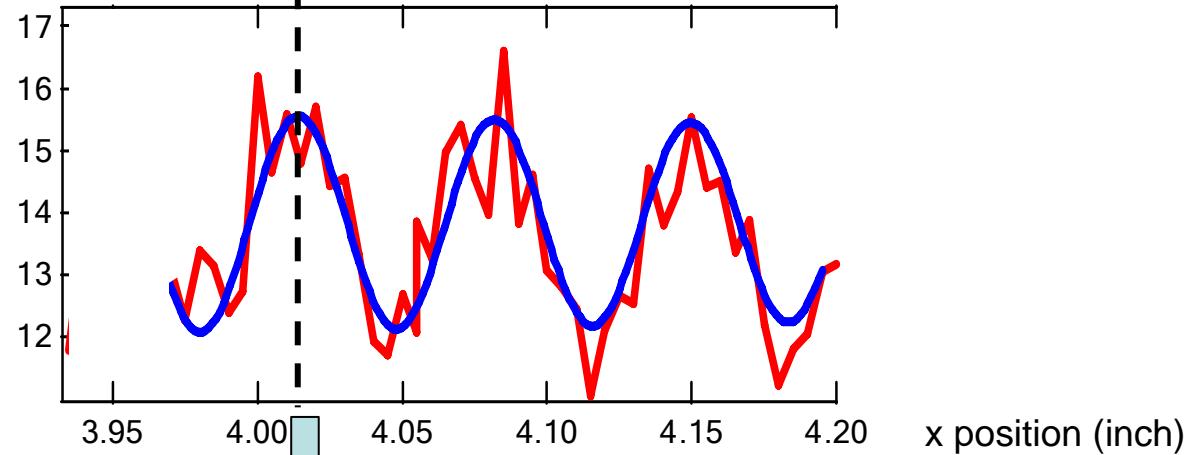


**RIXS with Standing Wave Excitation:
Fe-L x-ray emission, L₂ edge excitation at 722 eV
Cr-thickness (x-position) dependence**

Fe Int. =
 $I_{RCP} + I_{LCP}$
 \propto Total Fe

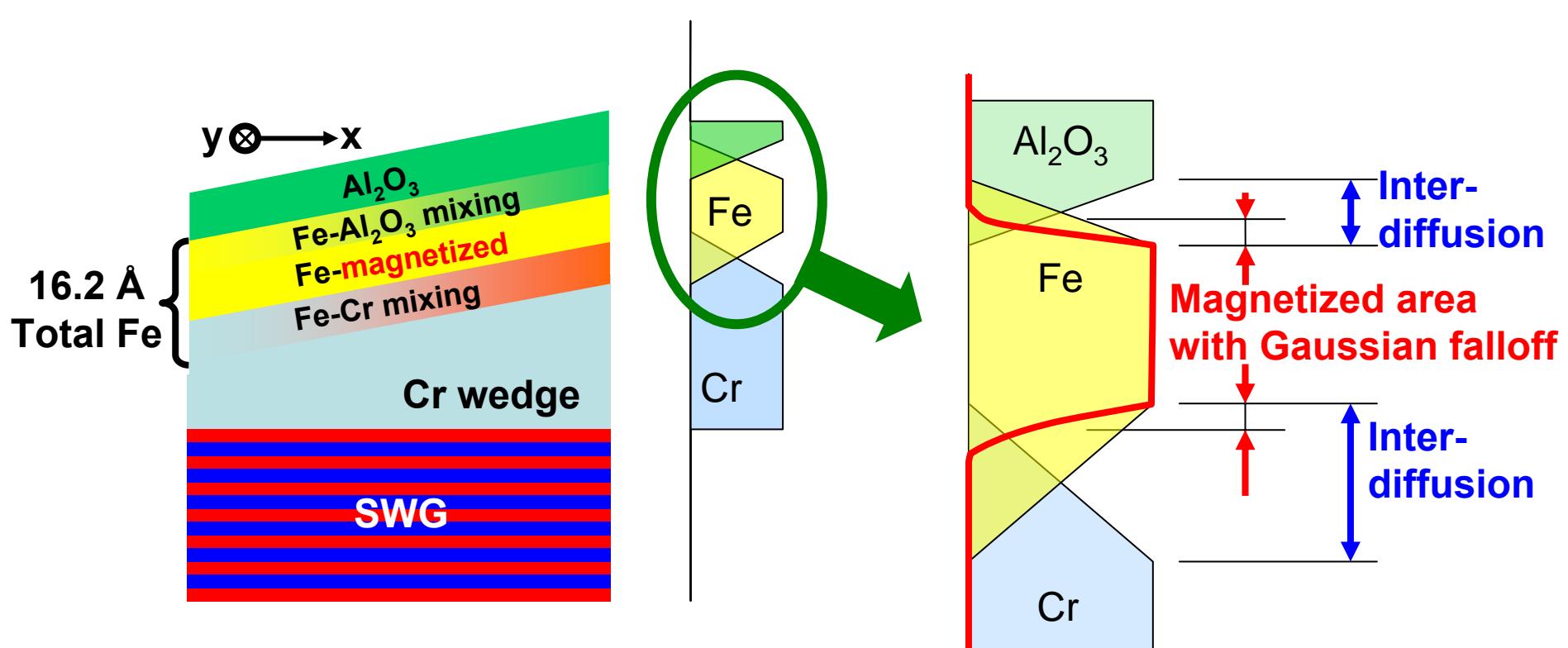


Fe MCD Asymmetry
 $\propto I_{RCP} - I_{LCP}$
 \propto Magnetized Fe

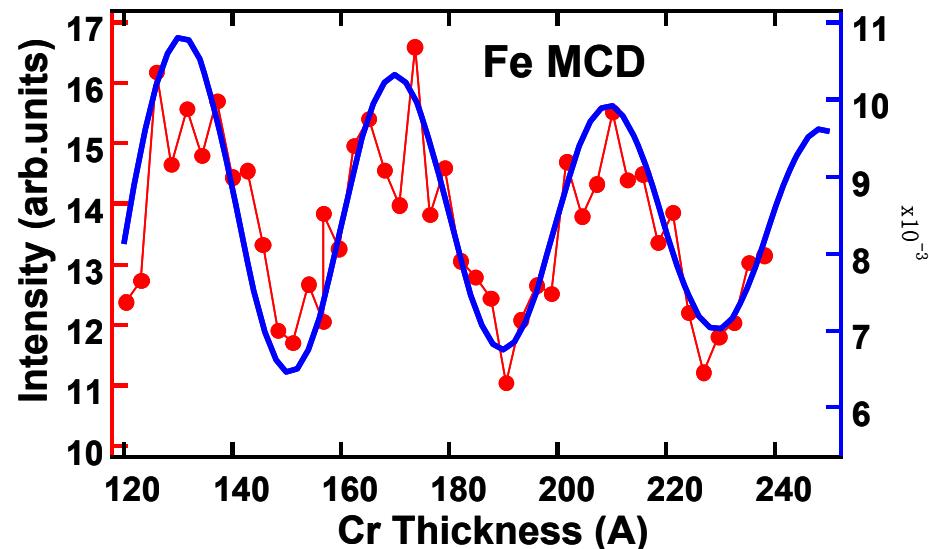
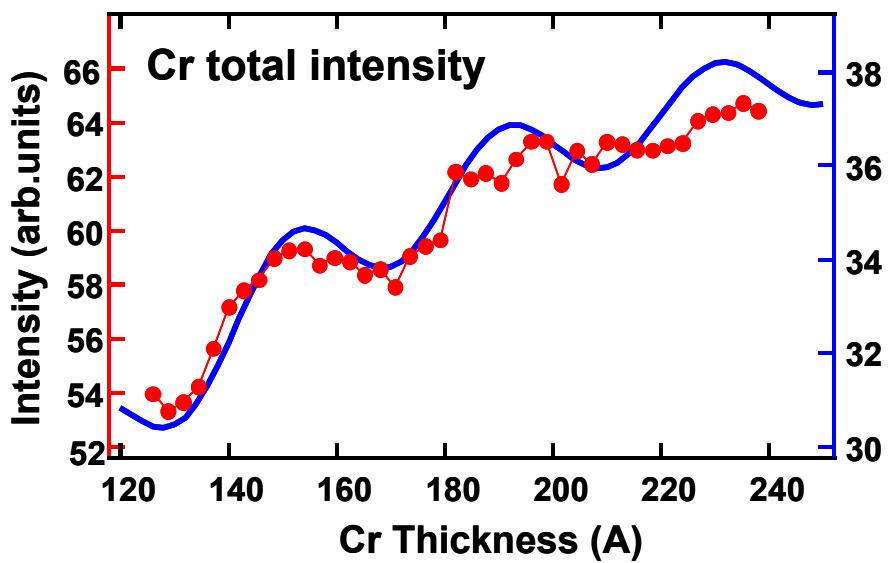
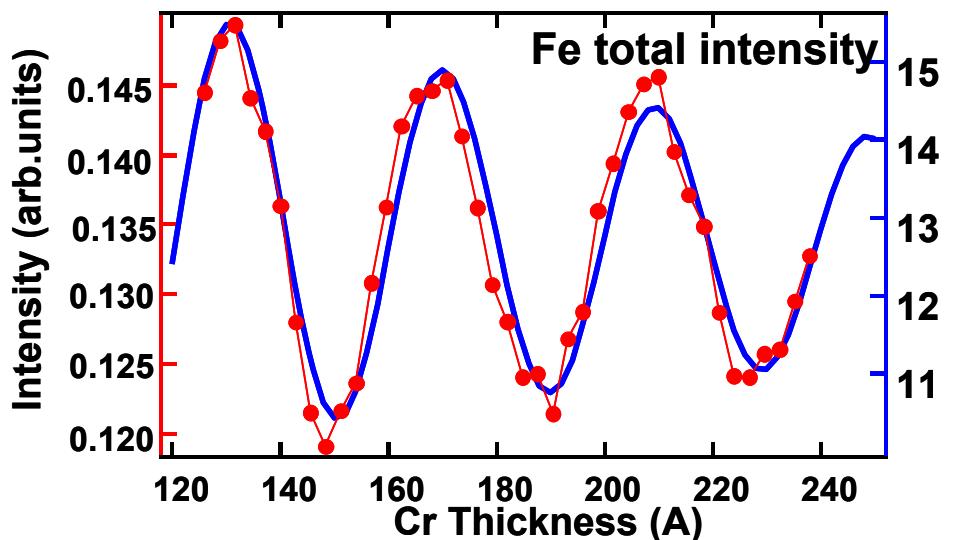
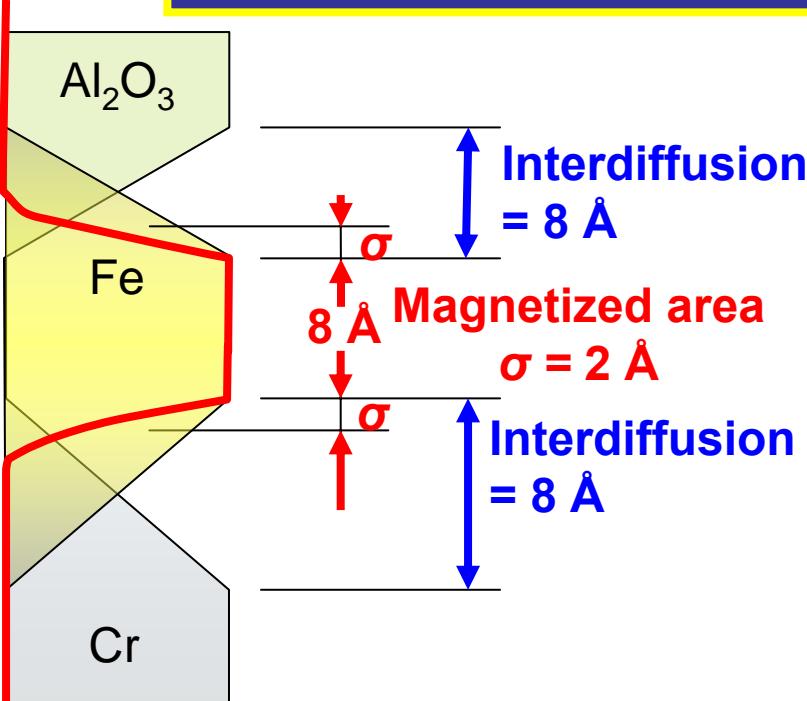


 No phase shift implies Total Fe and magnetized Fe at same average depth

X-ray Optical Modeling



XRO modeling: Al_2O_3 13Å / Fe 16.2Å / Cr 126-238Å / SWG



Standing Waves and Buried Layers/Interfaces

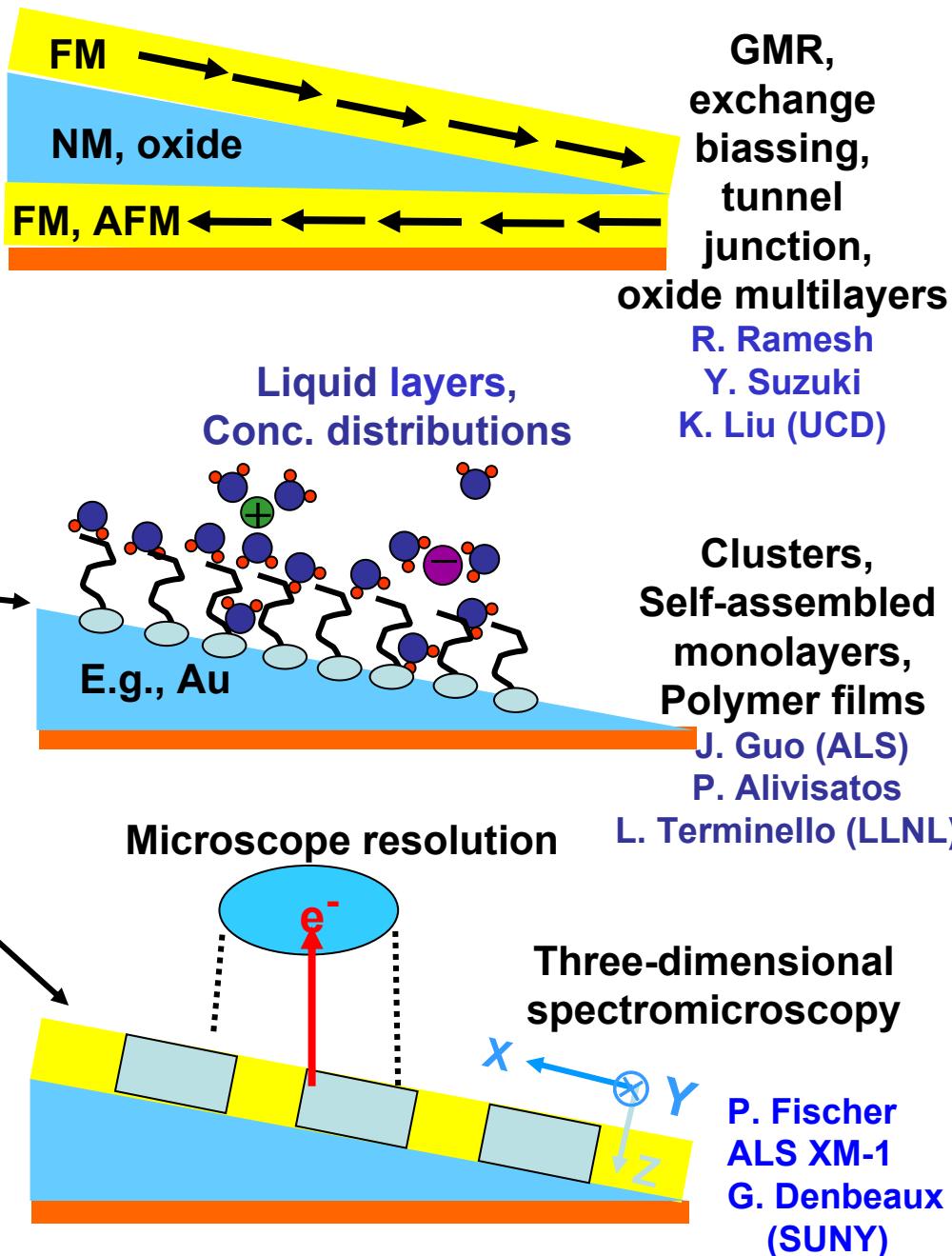
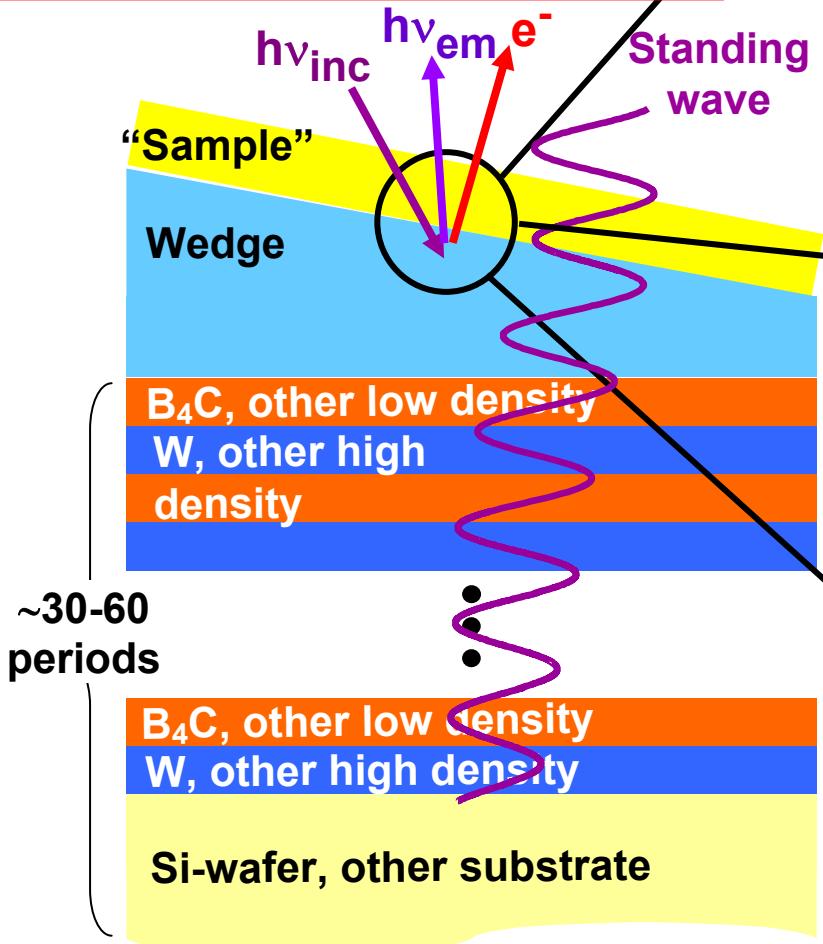
- Standing wave/wedge method—**electron-out**
Direct-space probing of various properties
Concentration and magnetization profiles (e.g. Fe/Cr)
Distribution of different chemical species (e.g. B in CoFeB, Co and Pt in CoPt alloy,...)
Layer-specific densities of states (e.g. CoFeB and CoFe)
- Standing wave/wedge method—**photon-out, deeper probe ~bulk**
First x-ray emission/RIXS results
Fe/Cr-wedge/multilayer--Fe-L $\alpha\beta$ +elastic intensities and MCD
Fe-Al₂O₃ and Fe-Cr interdiffusion at interfaces
- Data well reproduced by x-ray optical calculations—
Permits quantitative extraction of layer/interface properties
- Suggests many interesting future applications of approach with both **electron-out** and **photon-out** detection

Outline

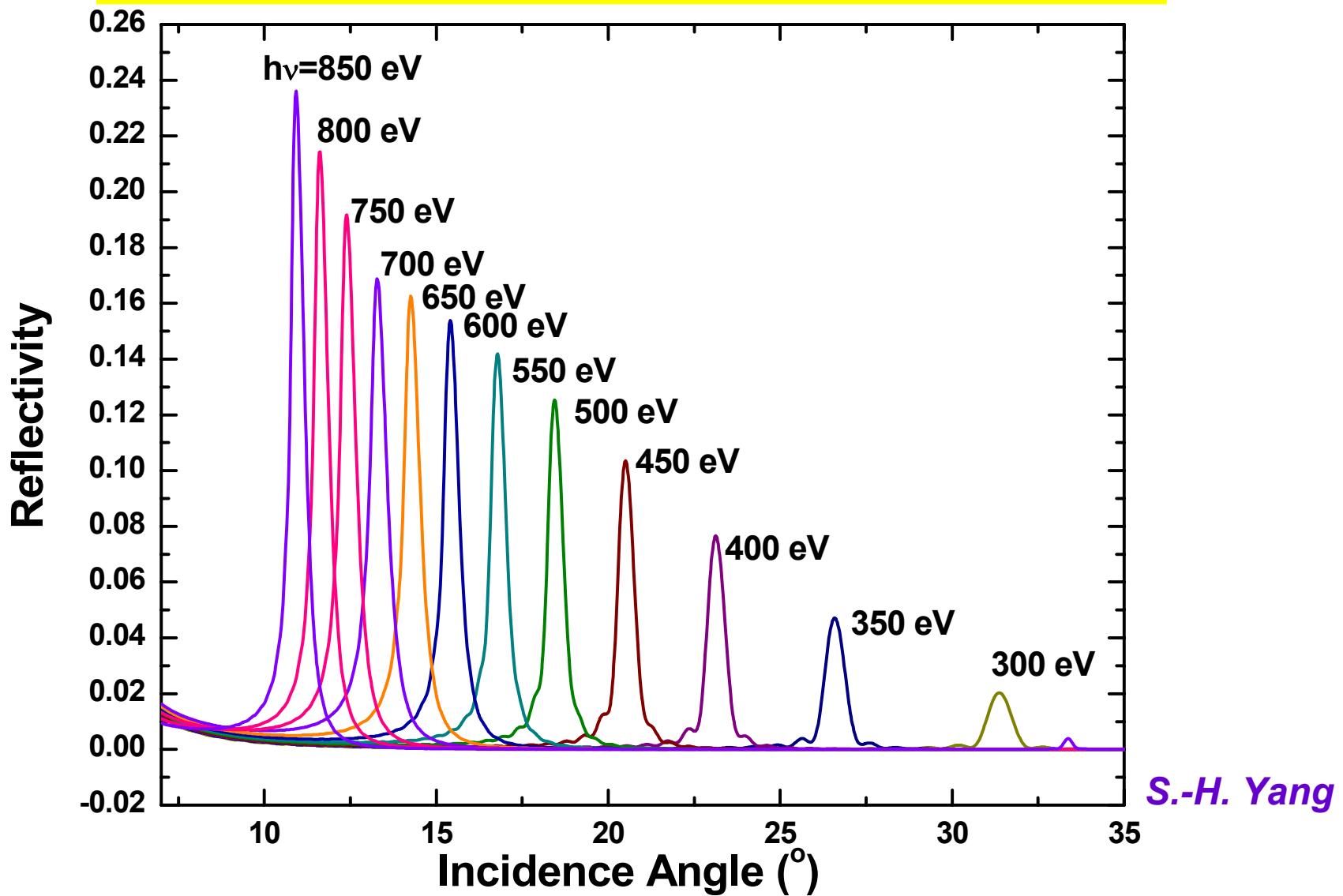
- Experimental aspects—end station on beamline 4.0.2
- Standing wave basics—rocking curves and wedges
- Photon-in/electron-out studies of spintronic nanolayer structures
- Photon-in/photon-out studies of spintronic nanolayer structures
- Future possibilities with photon-in/photon-out, including gas-solid and liquid-solid interfaces
- Resonant elastic soft x-ray scattering from nanostructures: Toward soft x-ray photonics?

STANDING-WAVE EXCITED SPECTROSCOPY--FUTURE POSSIBILITIES

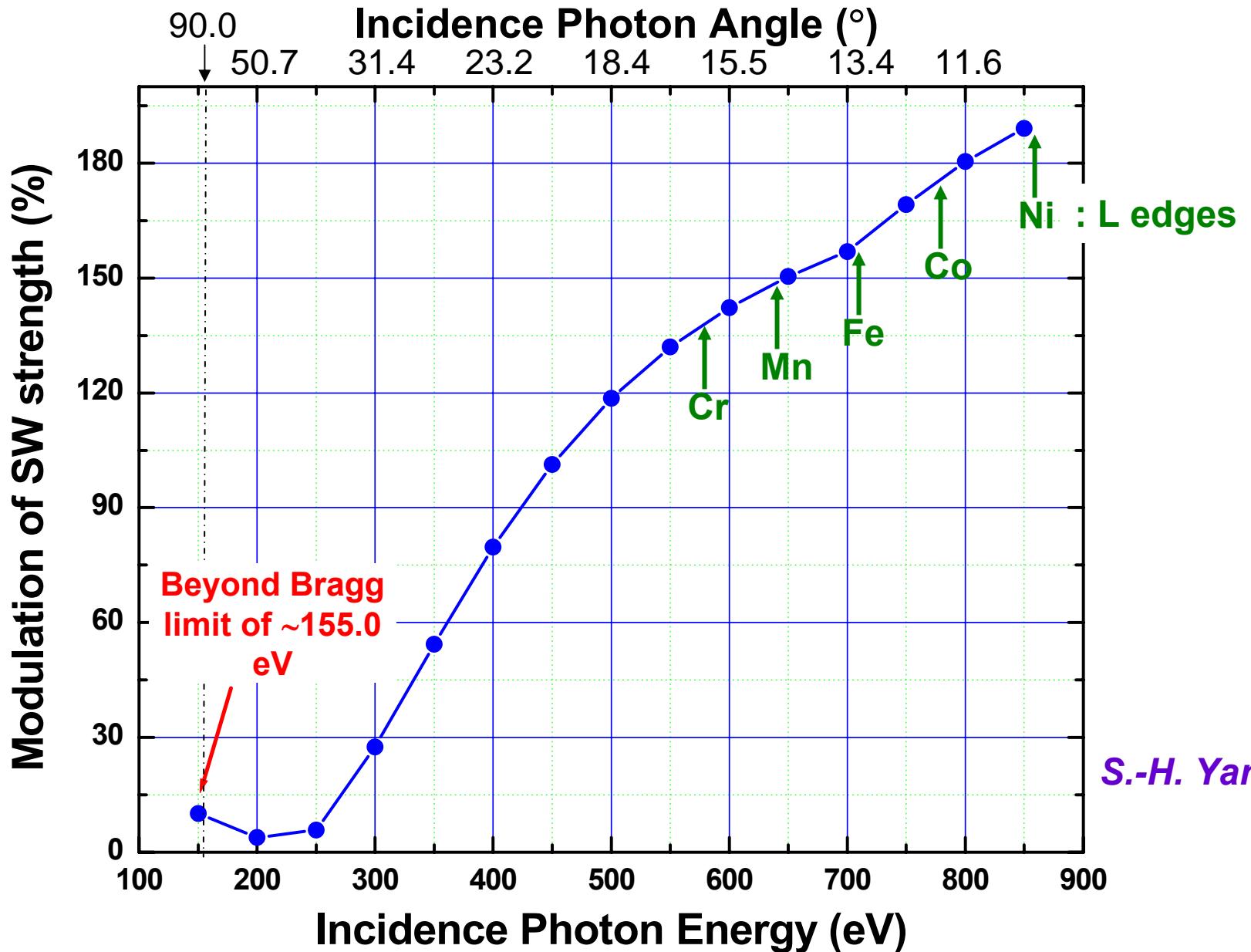
- Other material pairs in multilayer (B_4C/W , Al_2O_3/Pt , ...) + epitaxial multilayers → epitaxial samples
- Smaller periods (to ~25-30 Å) → smaller SW period, better resolution
- Lower $h\nu_{inc}$ → higher Bragg angles → perpend. component of M
- X-ray emission → deeper layers, more sensitivity to SW position



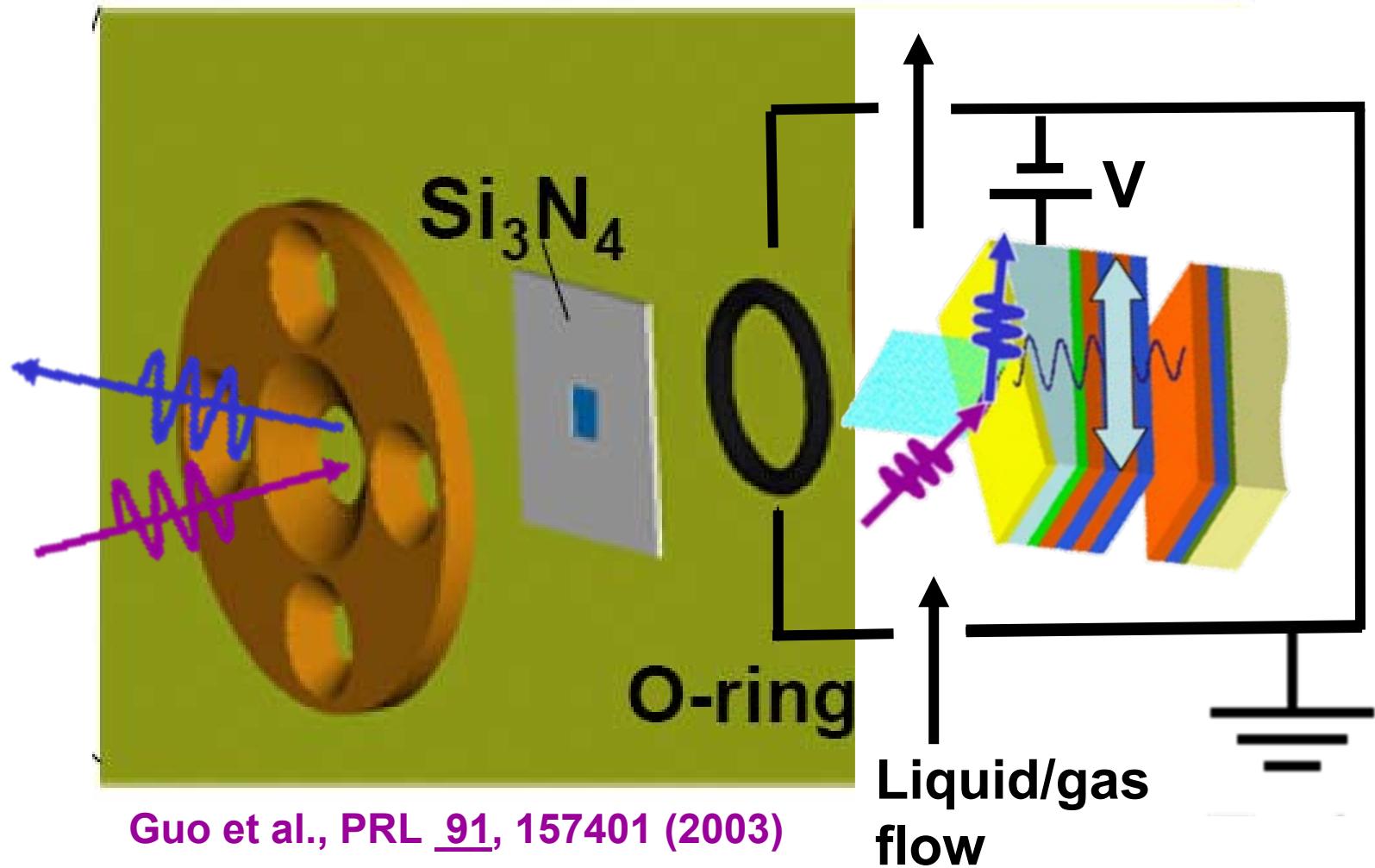
**Reflectivity for various photon energies
in $[B_4C$ (20 Å)/W (20 Å)]₄₀ ($h\nu = 300-850$ eV)**



**Modulation of SW $|E|^2$ at the shallowest bilayer
in $[B_4C\text{ (20 \AA)}/W\text{ (20 \AA)}]_{40}$**



XES/RIXS Studies in Real-World Conditions with Standing Wave Excitation



Guo et al., PRL 91, 157401 (2003)

Liquid/gas
flow

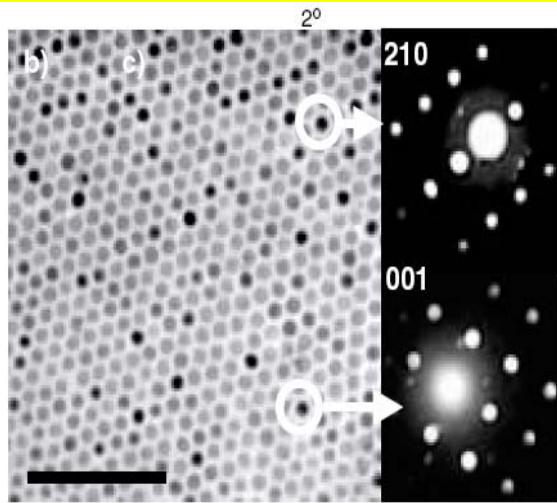
Guo, Fadley et al.

Outline

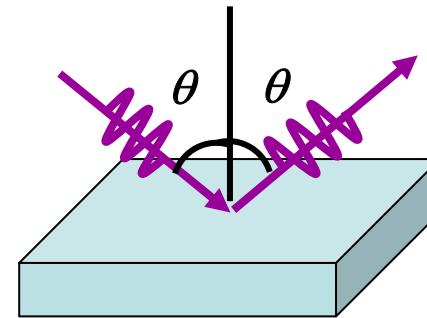
- Experimental aspects—end station on beamline 4.0.2
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Soft x-ray photonics?: 2D hcp array of Co nanoparticles

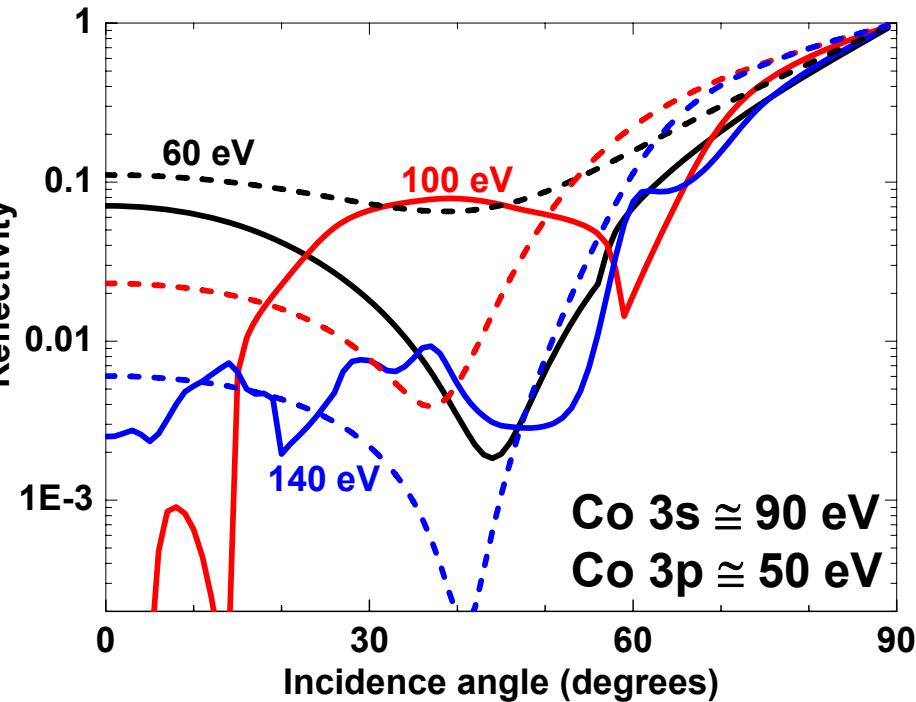
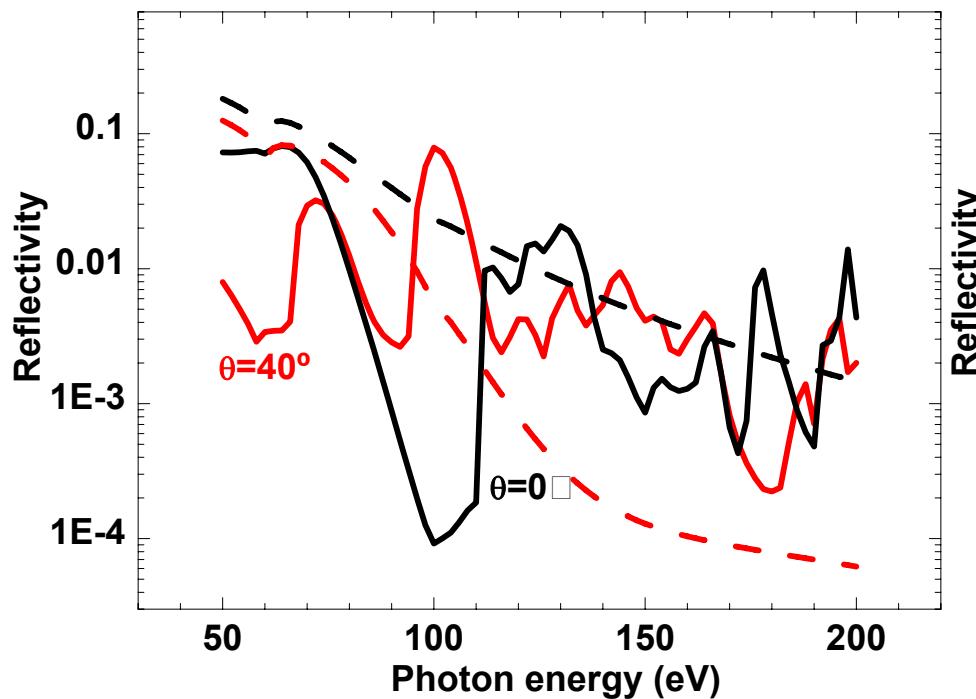
Puntes et al.,
Topics in Catal.
19, 145 (2002)



Theory: J. Garcia de Abajo:



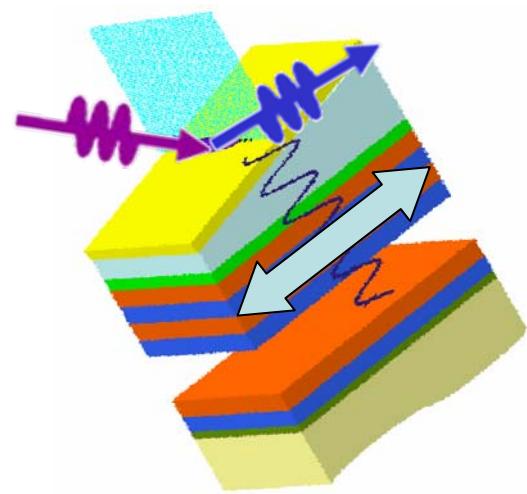
Solid curves—Co nanoarray
Dashed curves—flat surface of Co



Outline

- Experimental aspects—end station on beamline 4.0.2
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Finito



XRO modeling: Al_2O_3 13Å / Fe 16.2Å / Cr 126-238Å / SWG

